



# OpenGeoHub Summer School

# Mastering Machine Learning for Spatial Prediction I

## Practical training

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## Preparation

#### Load needed packages:

As an example you can work with the Berne soil mapping study area: dataset berne in R package geoGAM, contains continuous, binary and a multinomial/ordered response and a spatial data berne.grid for prediction.

Feel free to work with your own data!

Hint: The processing of this code is quite time consuming on a laptop. Normaly, one uses high performance computing facilities for machine learning.

Load the data, select the calibration set and remove missing values in covariates:

```
data(berne)
dim(berne)
## [1] 1052 238
# Continuous response
d.ph10 <- berne[berne$dataset == "calibration" & !is.na(berne$ph.0.10), ]
d.ph10 <- d.ph10[complete.cases(d.ph10[13:ncol(d.ph10)]), ]</pre>
# select validation data for subsequent validation
d.ph10.val <- berne[berne$dataset == "validation" & !is.na(berne$ph.0.10), ]</pre>
d.ph10.val <- d.ph10.val[complete.cases(d.ph10.val[13:ncol(d.ph10)]), ]</pre>
# Binary response
d.wlog100 <- berne[berne$dataset=="calibration"&!is.na(berne$waterlog.100), ]
d.wlog100 <- d.wlog100[complete.cases(d.wlog100[13:ncol(d.wlog100)]), ]</pre>
# Ordered/multinomial tesponse
d.drain <- berne[berne$dataset == "calibration" & !is.na(berne$dclass), ]</pre>
d.drain <- d.drain[complete.cases(d.drain[13:ncol(d.drain)]), ]</pre>
# covariates start at col 13
1.covar <- names(d.ph10[, 13:ncol(d.ph10)])</pre>
```

## 1 Lasso – linear shrinkage method

#### Lasso for continuous response

The berne dataset contains categorical covariates (factors, e.g. geological map with different substrate classes). The group lasso (R package grpreg) ensures that all dummy covariates of one factor are excluded (coefficients set to 0) together or remain in the model as a group.

The main tuning parameter  $\lambda$  is selected by cross validation.  $\lambda$  determines the degree of shrinkage that is applied to the coefficients.

HINT for R newbies: the apply-functions in R are replacements for loops (sapply: loop over a sequence of numbers, lapply: loop over a list). Compared to for, an apply is much faster and general coding style, though a bit more tricky to program.

Example, how to replace a for by a sapply:

```
# loop
# first create a vector to save the results
t.result <- c()
for( ii in 1:10 ){ t.result <- c(t.result, ii^2) }
# the same as apply
t.result <- sapply(1:10, function(ii){ ii^2 })</pre>
```

```
# of course, this example is even shorter using:
t.result <- (1:10)^2</pre>
```

Now we create the setup using apply and fit the grouped lasso:

```
# define groups: dummy coding of a factor is treated as group
# find factors
1.factors <- names(d.ph10[1.covar])[</pre>
  t.f <- unlist( lapply(d.ph10[l.covar], is.factor) ) ]</pre>
1.numeric <- names(t.f[ !t.f ])</pre>
# create a vector that labels the groups with the same number
g.groups <- c( 1:length(l.numeric),</pre>
               unlist(
                  sapply(1:length(l.factors), function(n){
                    rep(n+length(l.numeric), nlevels(d.ph10[, l.factors[n]])-1)
                  })
)
# grpreg needs model matrix as input
XX <- model.matrix(~., d.ph10[, c(l.numeric, l.factors), F])[,-1]
# cross validation (CV) to find lambda
ph.cvfit <- cv.grpreg(X = XX, y = d.ph10$ph.0.10,</pre>
                       group = g.groups,
                       penalty = "grLasso",
                       returnY = T) # access CV results
```

Compute predictions for the validation set with optimal number of groups chosen by lasso:

Get the lasso (non-zero) coefficients of the optimal model:

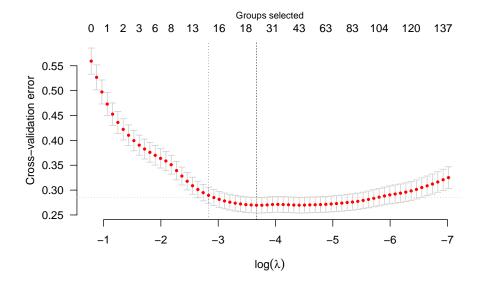


Figure 2: Cross validation error plotted against the tuning parameter lambda. The dashed line indicates lambda at minimal error, the dotted darkgrey line is the optimal lambda with minimal error + 1 SE.

```
##
                  9.734395e-05
                                               1.716402e-02
##
     tr_se_curvplan2m_std_25c
                                  tr_se_curvplan2m_std_50c
                  1.714450e-02
                                               2.037167e-03
##
                     tr_vdcn25
                                         timesetd1979_2010
##
##
                  1.064009e-03
                                               1.337349e-01
##
      timesetd1968_1974_field ge_geo500h3idTorfbedeckung
                  2.626367e-01
##
                                               1.061680e-01
```

#### Lasso for multinomial response

I am not aware of a lasso implementation for multinomial responses that can handle groups of factors. Therefore, we use "standard" lasso from R package glmnet (the option type.multinomial = "grouped" does only ensure all coefficients of the multinomial model for the same covariate are treated as groups).

For getting the coefficients of the final model you run the glmnet function again with the selected  $\lambda$ . Please note: The multinomial fit results in a coefficient for each covariate and response level.

#### Please continue:

- Select the lasso for a binary response (e.g. presence/absence of waterlogging waterlog.100). Use family = "binomial" in cv.grpreg and make sure your response is coded as 0/1.
- For the multinomial lasso fit of drainage class: compute predictions for the validation set (predict with s="lambda.1se" or s="lambda.min"). Then, evaluate prediction accuracy by e.g. using Pierce Skill Score, see function verify or multi.cont in R package verification.

## 2 Support vector machines

We use support vector machines (SVM) for regression from the package kernlab with radial kernel basis functions that fit local relations in feature space. The tuning parameter C defines the flexibility of the SVM to allow for wrongly predicted data points and the parameter  $\sigma$  the degree of non-linearity of the radial kernel. Here we apply a two step approach to find optimal tuning parameters. C and  $\sigma$  of a first pass are used as starting points to find optimal parameters around the first estimates.

We tune the SVM with caret with a cross-validation. caret is a meta package that provides a homogenous interface to about 80 machine learning methods.

```
# We have to set up the design matrix ourselfs
# (without intercept, hence remove first column)
XX <- model.matrix( ~., d.ph10[, c(l.covar), F])[,-1]</pre>
# set seed for random numbers to split cross-valiation sets
set.seed(31)
# Setup for 10fold cross-validation
ctrl <- trainControl(method="cv",</pre>
                     number=10,
                     savePredictions = "final")
# 1. pass of training - find region of C and lambda
svm.tune1 \leftarrow train(x = XX,
                   y = d.ph10[, "ph.0.10"],
                   method = "svmRadial", # radial kernel function
                   tuneLength = 9, # check 9 values of the cost function
                   preProc = c("center", "scale"), # center and scale data
                   trControl=ctrl)
# 2. pass of training - find best value for C and lambda
# setup a tuning grid with values around the result of the first pass
sig <- svm.tune1$bestTune$sigma</pre>
t.sigma <- sort( unique( round(abs( c(sig, sig + seq(0, sig*2, by = sig/1),
                                       sig - seq(0, sig*2, by = sig/1))), 6)))
tune.grid <- expand.grid(</pre>
  sigma = t.sigma[t.sigma>0], # sigma must be positive
  C = sort( unique( abs( c(svm.tune1$bestTune$C,
                            svm.tune1$bestTune$C - seq(0, 0.3, by = 0.1),
                            svm.tune1$bestTune$C + seq(0, 0.3, by = 0.1))))
#Train and Tune the SVM
svm.model <- train(x = XX,</pre>
                   y = d.ph10[, "ph.0.10"],
                   method = "svmRadial",
                   preProc = c("center", "scale"),
                   tuneGrid = tune.grid,
                   trControl = ctrl)
# -> if this takes too long: take a short cut with
# svm.model <- svm.tune1
```

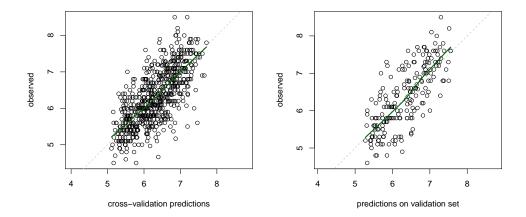


Figure 3: Predictions from cross-validation (left) and the validation dataset (right) plotted against the observed values (dashed: 1:1-line, green: lowess scatterplott smoother).

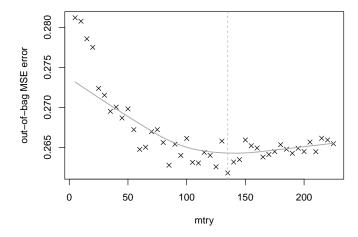
```
# create validation plots with lowess scatterplot smoothers
# for cross-validation
par(mfrow = c(1,2))
plot(svm.model$pred$pred, svm.model$pred$obs,
     xlab = "cross-validation predictions",
     ylab = "observed",
     asp = 1)
abline(0,1, lty = "dashed", col = "grey")
lines(lowess(svm.model$pred$pred, svm.model$pred$obs), col = "darkgreen", lwd = 2)
# for independent validation set
# calculate predictions for the validation set
newXX <- model.matrix( ~., d.ph10.val[, l.covar, F])[,-1]</pre>
t.pred.val <- predict.train(svm.model, newdata = newXX)</pre>
plot(t.pred.val, d.ph10.val[, "ph.0.10"],
     xlab = "predictions on validation set",
     ylab = "observed",
     asp = 1
abline(0,1, lty = "dashed", col = "grey")
lines(lowess(t.pred.val, d.ph10.val[, "ph.0.10"]), col = "darkgreen", lwd = 2)
```

#### 3 Random forest

Here we fit a random forest with the package ranger, a fast implementation of this algorithm for large data sets. More important: use parallel computing as demonstrated here e.g. with the function mclapply (does not work on Windows, then use mc.cores = 1).

This is advanced programming with functions and apply. But, I wanted to show how you can do the tuning of a ML method yourself without using a meta-function like train from package caret (see below). Like this you can control that it does what you acctually want to achieve (and the code is not much longer)

```
# Fit a random forest with default parameters
# (often results are already quite good)
set.seed(1)
rf.model.basic <- ranger(x = d.ph10[, 1.covar ],</pre>
                         y = d.ph10[, "ph.0.10"])
# tune main tuning parameter "mtry"
# (the number of covariates that are randomly selected to try at each split)
# define function to use below
f.tune.randomforest <- function(test.mtry, # mtry to test</pre>
                                 d.cal,
                                          # calibration data.frame
                                 1.covariates ){ # list of covariates
  # set seed
  set.seed(1)
  # fit random forest with mtry = test.mtry
  rf.tune <- ranger(x = d.cal[, l.covariates ],</pre>
                    y = d.cal[, "ph.0.10"],
                    mtry = test.mtry)
  # return the mean squared error (mse) of this model fit
  return( rf.tune$prediction.error )
# vector of mtry to test
seq.mtry <- 1:(length(l.covar) - 1)</pre>
# Only take every fifth mtry to speed up tuning
seq.mtry <- seq.mtry[ seq.mtry %% 5 == 0 ]</pre>
# Apply function to sequence.
system.time(
 t.00Be <- mclapply(seq.mtry, # give sequence
                       FUN = f.tune.randomforest, # give function name
                       mc.cores = 1, ## number of CPUs
                       mc.set.seed = FALSE, # do not use new seed each time
                       # now here giv the arguments to the function:
                       d.cal = d.ph10,
                       1.covar = 1.covar )
)
##
      user system elapsed
## 768.113 0.703 104.794
```



**Figure 4:** Tuning parameter mtry plotted against the out-of-bag mean squared error (grey line: lowess smoothing line, dashed line: mtry at minimum MSE).

#### Please continue:

- Compute the predictions for the validation set with the tuned and the model with default values (predict(rf.model.tuned, newdata = ...)) and compute a root mean squared error. Was the tuning effort worthwhile?
- Implement the same tunging with the package caret. Check the option method="oob" of trainControl. This function is handed to train.

## 4 Gradient boosting

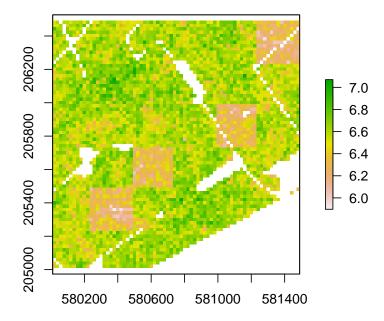
#### 4.1 Boosting with trees as baselearners

There are various R packages to fit boosting models (e.g. mboost, xgboost). We use gbm here. We can again tune it with caret. caret is a meta package that provides a homogenous interface to about 80 machine learning methods.

Fit gradient boosting with trees:

```
# create a grid of the tuning parameters to be tested,
# main tuning parameters are:
gbm.grid <- expand.grid(</pre>
  # how many splits does each tree have
 interaction.depth = c(2,5,10,15,20),
  # how many trees do we add (number of iterations of boosting algorithm)
 n.trees = seq(2,250, by = 5),
  # put the shrinkage factor to 0.1 (=10% updates as used
  # in package mboost), the default (0.1%) is a bit too small,
  # makes model selection too slow.
  # minimum number of observations per node can be left as is
 shrinkage = 0.1, n.minobsinnode = 10)
# make tuning reproducible (there are random samples for the cross validation)
set.seed(291201945)
# train the qbm model
# Remove "qe_caco3" throws an error since Package qbm 2.1.5,
# this bug is reported: https://github.com/qbm-developers/qbm/issues/40
gbm.model \leftarrow train(x=d.ph10[, 1.covar[-c(50)]],
                   y=d.ph10[, "ph.0.10"],
                   method = "gbm", # choose "generalized boosted regression model"
                   tuneGrid = gbm.grid,
                   verbose = FALSE,
                   trControl = trainControl(
                     # use 10fold cross validation (CV)
                     method = "cv", number = 10,
                     # save fitted values (e.g. to calculate RMSE of the CV)
                     savePredictions = "final"))
# print optimal tuning parameter
gbm.model$bestTune
##
     n.trees interaction.depth shrinkage n.minobsinnode
## 24 117
                              2
                                0.1
# compute predictions for the small part of the study area
# (agricultural land, the empty pixels are streets, forests etc.)
data("berne.grid")
```

berne.grid\$pred <- predict.train(gbm.model, newdata = berne.grid )</pre>



**Figure 5:** Predictions computed with an optimized boosted trees model of topsoil pH (0–10 cm) for a very small part of the Berne study region (white areas are streets, developped areas or forests, CRAN does not accept larger datasets).

```
# create a spatial object for a proper spatial plot
coordinates(berne.grid) <- ~x+y
# add the Swiss projection (see ?berne.grid)
# see https://epsg.io for details on projections
proj4string(berne.grid) <- CRS("+init=epsg:21781")
# create a raster object from the spatial point dataframe
gridded(berne.grid) <- TRUE
plot(raster(berne.grid, layer = "pred"))</pre>
```

Lets check the partial dependencies of the 4 most important covariates:

```
# get variable importance
t.imp <- varImp(gbm.model$finalModel)

# check how many covariates were never selected
sum( t.imp$Overall == 0 )

## [1] 111

# order and select 4 most important covariates
t.names <- dimnames(t.imp)[[1]][ order(t.imp$Overall, decreasing = T)[1:4] ]

par(mfrow = c(2,2))
for( name in t.names ){</pre>
```

```
# select index of covariate
ix <- which( gbm.model$finalModel$var.names == name )
plot(gbm.model$finalModel, i.var = ix)
}

# -> improve the plots by using the same y-axis (e.g. ylim=c(..,..))
# for all of them, and try to add labels (xlab = , ylab = )
# or a title (main = )
```

#### 4.2 Boosting with linear baselearners (advanced task)

Boosting algorithm can be used with any kind of base procedures / baselearners. Many packages (e.g. gbm, xgboost) use trees. Here we try linear and splines baselearners.

For details on mboost see the hands-on tutorial in the vignette to the package: https://cran.r-project.org/web/packages/mboost/vignettes/mboost\_tutorial.pdf

Select a boosting model with linear baselearners (this results in shrunken coefficients, similar to the lasso, see Hastie et al. 2009):

#### 4.3 Boosting with splines baselearners (advanced task)

To model non-linear relationships we use splines baselearners. Spatial autocorrelation can be captured by adding a smooth spatial surface. This type of model needs a bit more setup. Each covariate type has its own specification. All baselearners should have the same degrees of freedom, otherwise biased model selection might be the result.

```
# quick set up formula

# Response
f.resp <- "ph.0.10 ~ "</pre>
```

#### 10-fold kfold

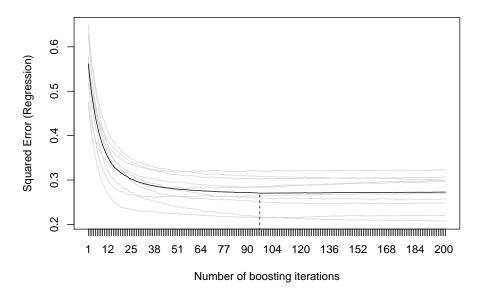


Figure 6: Path of cross validation error along the boosting iterations.

```
# Intercept, add to dataframe
f.int <- "bols(int, intercept = F, df = 1)"</pre>
d.ph10$int <- rep(1, nrow(d.ph10))</pre>
# Smooth spatial surface (needs > 4 degrees of freedom)
f.spat \leftarrow "bspatial(x, y, df = 5, knots = 12)"
# Linear baselearners for factors, maybe use df = 5
f.fact <- paste(</pre>
  paste( "bols(", l.factors, ", intercept = F)" ),
  collapse = "+"
)
# Splines baselearners for continuous covariates
f.num <- paste(</pre>
  paste( "bbs(", l.numeric, ", center = T, df = 5)" ),
  collapse = "+"
# create complete formula
ph.form <- as.formula( paste( f.resp,</pre>
                                paste( c(f.int, f.num, f.spat, f.fact),
                                        collapse = "+")) )
# fit the boosting model
ph.gamboost <- gamboost(ph.form, data = d.ph10,</pre>
                           control = boost_control(mstop = 200))
# Find tuning parameter
ph.gamboost.cv <- cvrisk(ph.gamboost,</pre>
```

#### Analyse boosting model:

```
# print optimal mstop
mstop(ph.gamboost.cv)
## [1] 192
## print model info
ph.gamboost[ mstop(ph.glmboost.cv)]
##
##
     Model-based Boosting
##
## Call:
   gamboost(formula = ph.form, data = d.ph10, control = boost_control(mstop = 200))
##
##
##
     Squared Error (Regression)
##
## Loss function: (y - f)^2
##
##
## Number of boosting iterations: mstop = 96
## Step size: 0.1
## Offset: 6.314042
## Number of baselearners:
## print number of chosen baselearners
length( t.sel <- summary( ph.gamboost[ mstop(ph.glmboost.cv)] )$selprob )</pre>
## [1] 33
# Most often selected were:
summary( ph.gamboost[ mstop(ph.glmboost.cv)] )$selprob[1:5]
##
                      bols(timeset, intercept = F)
##
                                         0.14583333
               bbs(cl_mt_gh_3, df = 5, center = T)
##
##
                                         0.08333333
           bbs(tr_ch_3_80_10s, df = 5, center = T)
##
##
                                         0.06250000
               bbs(cl_mt_gh_8, df = 5, center = T)
##
##
                                         0.05208333
## bbs(tr_be_twi2m_s60_tcilow, df = 5, center = T)
##
```

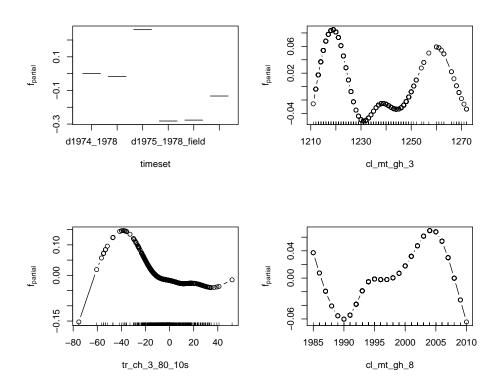
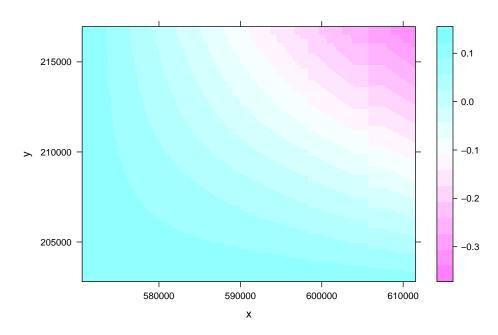


Figure 7: Residual plots of the 4 covariates with highest selection frequency.



 ${\bf Figure~8:~} {\bf Modelled~smooth~spatial~surface~based~on~the~coordinates.}$ 

## 5 Model averaging

So far we calibrated several models to predict topsoil pH. With model averaging we can combine these predictions computing a simple mean. Besides simple averaging, we could use weights like  $\frac{1}{MSE}$  (make sure they sum up to 1).

Compute validation statistics (e.g. root mean squared error,  $R^2$ ) on the validation set for the predictions of each model and the (weighted) averaged predictions. Is the prediction accuracy improved?

You could now add models computed from random forest, support vector machines or gradient boosted trees. Does this improve model accuracy?

Note: Be aware not to select the final model based on the validation data. If you start tuning your predictions on your validation data, you loose the independent estimate of prediction accuracy... better choose your method for the final predictions based on cross validation (e.g. on the same sets).

### R session information

This document was generated with:

```
toLatex(sessionInfo(), locale = FALSE)
```

- R version 3.5.0 (2018-04-23), x86\_64-pc-linux-gnu
- Running under: Progress Linux 4+ (dschinn-backports)
- Matrix products: default
- BLAS: /usr/lib/openblas-base/libblas.so.3
- LAPACK: /usr/lib/libopenblasp-r0.2.19.so
- Base packages: base, datasets, graphics, grDevices, methods, parallel, stats, utils
- Other packages: caret 6.0-81, foreach 1.4.4, gbm 2.1.4, geoGAM 0.1-2, ggplot2 3.1.1, glmnet 2.0-16, grpreg 3.2-0, kernlab 0.9-27, knitr 1.20, lattice 0.20-38, Matrix 1.2-15, mboost 2.9-1, quantregForest 1.3-7, randomForest 4.6-14, raster 2.8-4, RColorBrewer 1.1-2, sp 1.3-1, stabs 0.6-3
- Loaded via a namespace (and not attached): assertthat 0.2.1, bindr 0.1.1, bindrcpp 0.2.2, class 7.3-14, codetools 0.2-15, colorspace 1.4-1, compiler 3.5.0, crayon 1.3.4, data.table 1.11.8, digest 0.6.18, dplyr 0.7.8, evaluate 0.12, Formula 1.2-3, generics 0.0.1, glue 1.3.1, gower 0.1.2, grid 3.5.0, gridExtra 2.3, gtable 0.3.0, highr 0.7, inum 1.0-0, ipred 0.9-8, iterators 1.0.10, lava 1.6.4, lazyeval 0.2.2, libcoin 1.0-1, lubridate 1.7.4, magrittr 1.5, MASS 7.3-51.1, mgcv 1.8-25, ModelMetrics 1.2.2, munsell 0.5.0, mvtnorm 1.0-8, nlme 3.1-137, nnet 7.3-12, nnls 1.4, partykit 1.2-2, pillar 1.3.1, pkgconfig 2.0.2, plyr 1.8.4, prodlim 2018.04.18, purrr 0.2.5, quadprog 1.5-5, R6 2.4.0, Rcpp 1.0.1, recipes 0.1.4, reshape2 1.4.3, rgdal 1.3-6, rlang 0.3.4, rpart 4.1-13, rstudioapi 0.8, scales 1.0.0, splines 3.5.0, stats4 3.5.0, stringi 1.4.3, stringr 1.4.0, survival 2.43-1, tibble 2.1.1, tidyselect 0.2.5, timeDate 3043.102, tools 3.5.0, withr 2.1.2

```
##
##
##
## processing file: OpenGeoHub-machine-learning-training-1.Rnw
## Error in parse_block(g[-1], g[1], params.src): duplicate label 'general-options'
```