Machine learning methods for soil mapping: Random Forest Modelling

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Machine learning

- No clear definition among experts.
- Machine learning is a “field of computer science that gives computers the ability to learn without being explicitly programmed” (Samuel, 1959).
- Ability to “learn” (supervised, unsupervised); self-driving cars, email filtering, web search, image recognition (incl. faces).
- Uncovering patterns and structures in (large) data sets; deriving predictive relationships, which makes machine learning algorithms interesting for digital soil mapping.

Algorithms: Random Forest

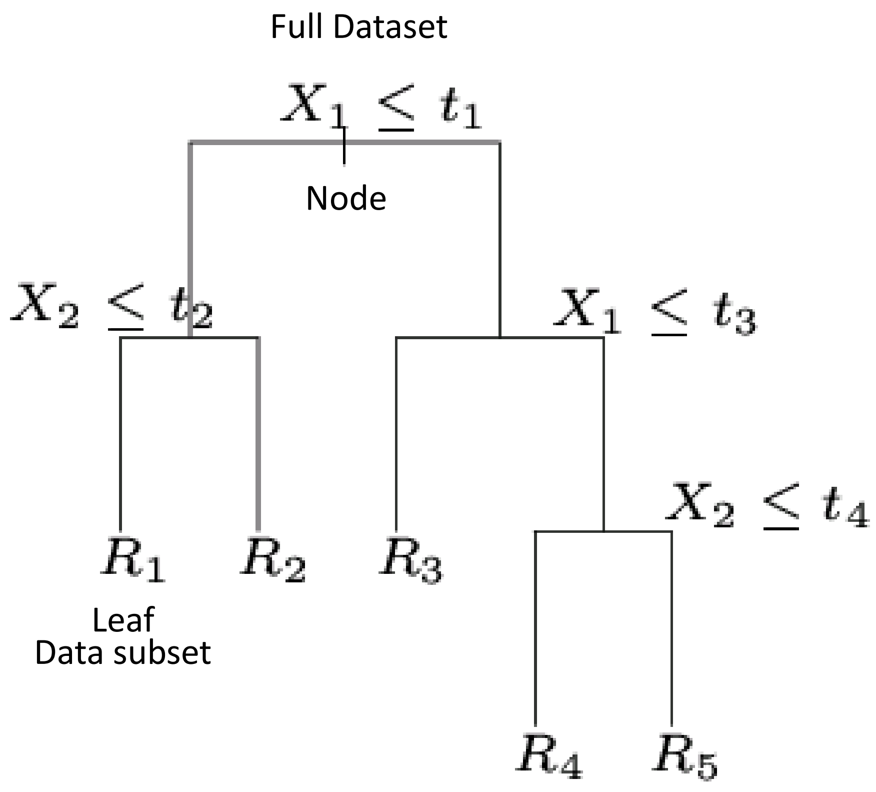
- Many algorithms: **random forest**, neural nets, gradient boosting and many more.
- Machine learning algorithms have become very popular for digital soil mapping since the last 5 years or so, especially random forest modelling.
- Random Forest developed by Tin Kam Ho (1995) and Leo Breiman (2001).
- Based on decision tree models.
- Let’s take a look at these first.

Classification and regression trees (CART)

- Classification tree for categorical data
- Regression tree for continuous data
- Overcome limitations of classical (linear) model:
  - non-linear relationships;
  - n of covariates > n observations;
  - interactions of categorical covariates that result in sparse cell counts;
  - non-parametric.
- Tree modelling: recursive partitioning of the data based on binary splitting using covariates

Growing a tree model

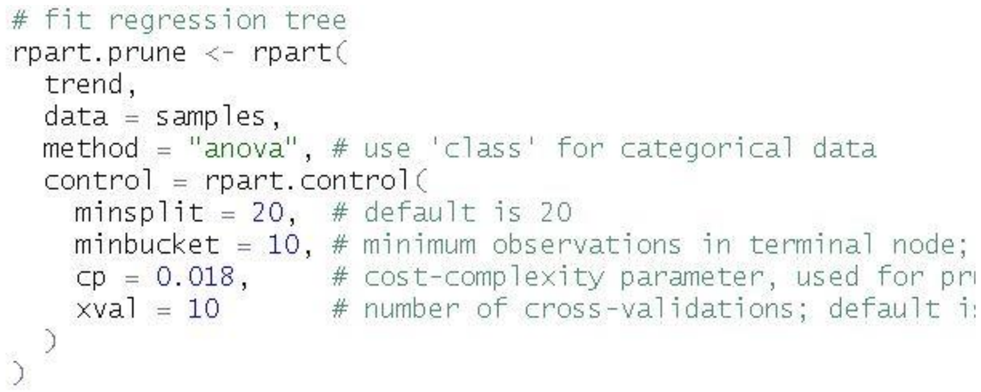
- Evaluate all covariates for each split.
- Split is chosen so that a maximum reduction of the error is achieved. Each node is more 'pure' than its parent node.
- Splitting process is repeated for next two nodes, etc.
- Greedy algorithm.
- The prediction at a leaf is the **mean** value of the data points (RT) or the **modal** class (CT).



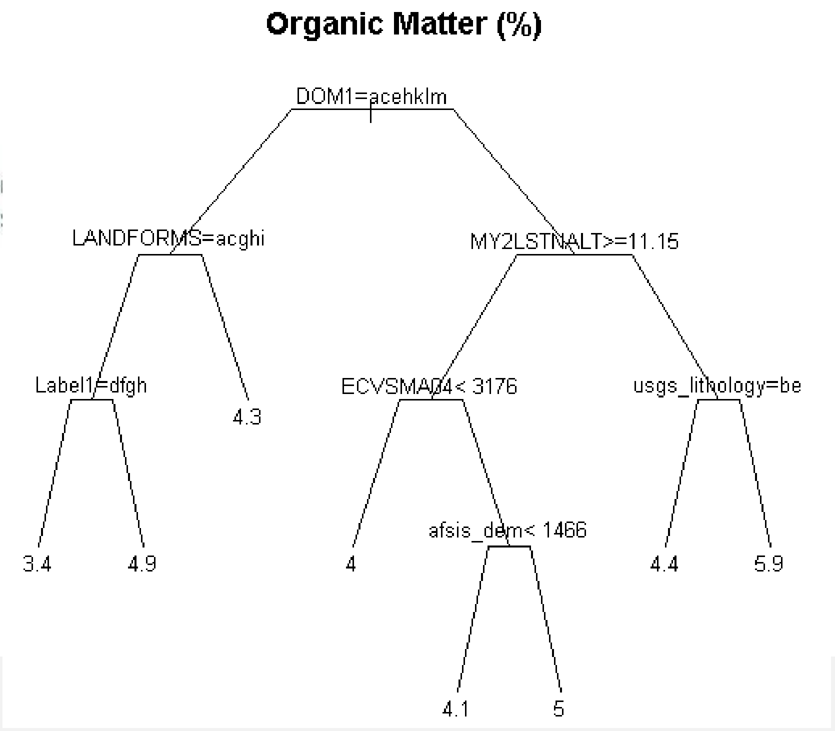
Source: Hastie et al., 2009. The Elements of Statistical Learning

Growing a tree in R

- rpart, tree, party packages
- Fitting a tree model to soil organic matter content



```
# fit regression tree
rpart.prune <- rpart(
  trend,
  data = samples,
  method = "anova", # use 'class' for categorical data
  control = rpart.control(
    minsplit = 20,  # default is 20
    minbucket = 10, # minimum observations in terminal node;
    cp = 0.018,     # cost-complexity parameter, used for pr
    xval = 10       # number of cross-validations; default i:
  )
)
```



Random Forests

- Limitations of CART:
  - Trees are known to be instable: sensitive to small changes in learning data -> tree structure can be completely altered.
  - Predictions of single trees show high variability: trees built on different bootstrap samples can have different structures.
  - Danger of over-fitting.
- Can be avoided using **ensemble methods**: base prediction on a whole set of trees rather than a single tree
- Ensemble methods use the fact that individual trees are unstable but on average produce the right result.
- Random forests is such ensemble method: a forest of trees is grown; the prediction is an aggregation of the individual tree predictions.

How does it work?

- Random forests combine:
  - bootstrap aggregation (‘bagging’)
  - random selection of predictors
- Algorithm:
  - Draw a bootstrap sample:
    - Random selection of 2/3 of the training data; repeat *n* times.
    - Grow an unpruned tree to each bootstrap sample
  - Random predictor selection: for each split in each tree a random subset is selected from the predictor variables. The best split is chosen from among the selected predictors.
  - Predict new data by aggregating the predictions of the n trees.
    - Average for continuous variables
    - Majority vote for categorical variables.

Fitting a random forest model

- Training data (soil property of interest)
- Explanatory variables (environmental covariates)
- Model tuning parameters:
  - **mtry**: number of randomly selected splitting variables.
  - **ntree**: number of trees grown
- Choice of mtry and ntree parameters affect the stability of the tree:
  - Should be large enough so that each variable has a chance to occur in enough trees
  - Adjust if prediction results and variable importance differ for different random seeds
  - Optimize tuning parameters (with caret package)

Out-Of-Bag accuracy assessment

- Random Forest comes with an internal accuracy assessment (based on cross-validation; no need to do a separate assessment).

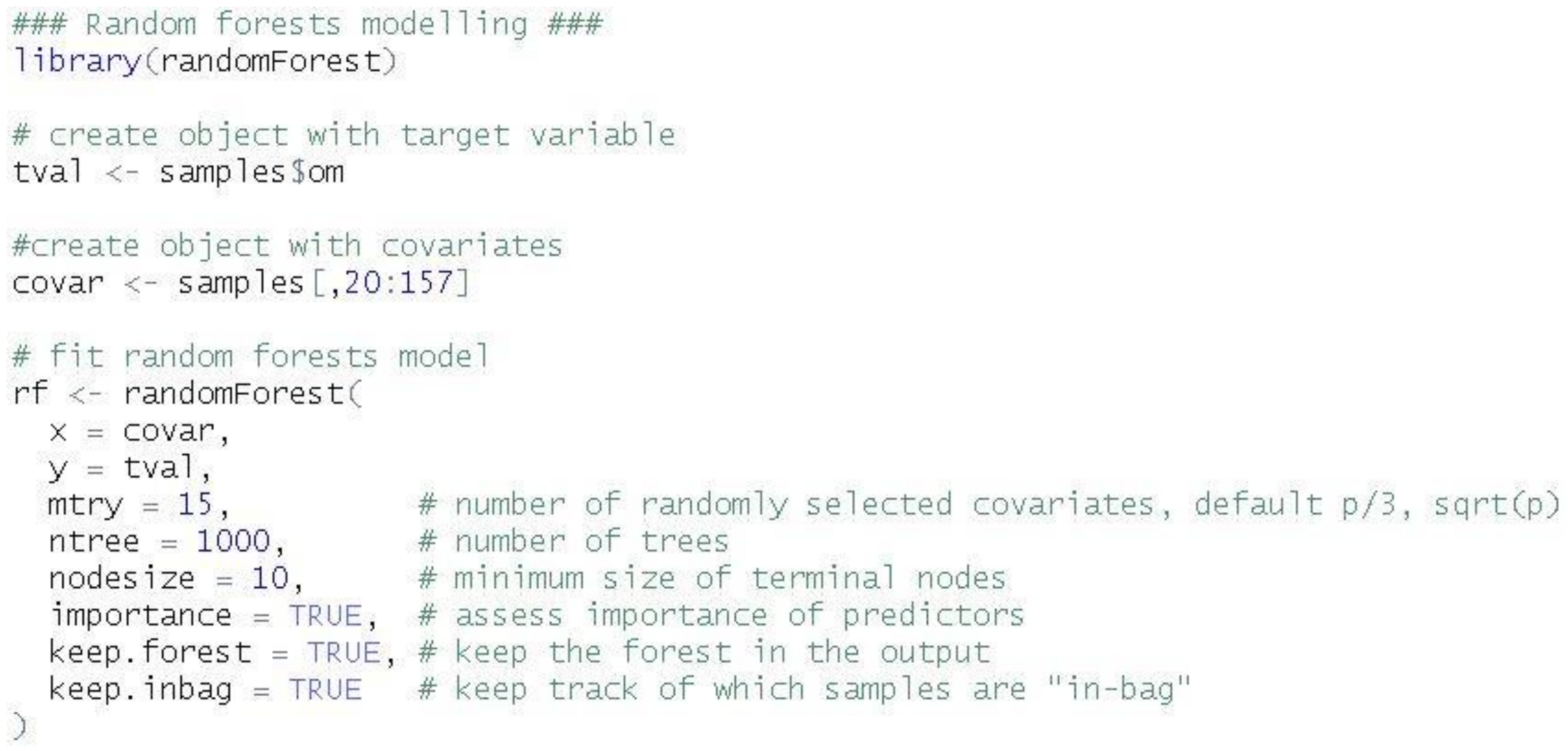
- Bootstrap sampling: the algorithm sets aside ~36% of the training data for each tree grown: out-of-bag data (OOB).

- Each data point will be OOB for approximately ~36% of the number of fitted trees.

- OOB data can be used to asses prediction accuracy:
  - Predict the data not in the bootstrap sample for each tree
  - Aggregate the OOB predictions: **mean** (continuous data), **majority vote** (categorical data).

Application in R

- Packages: **randomForest**, ranger, cforest, party



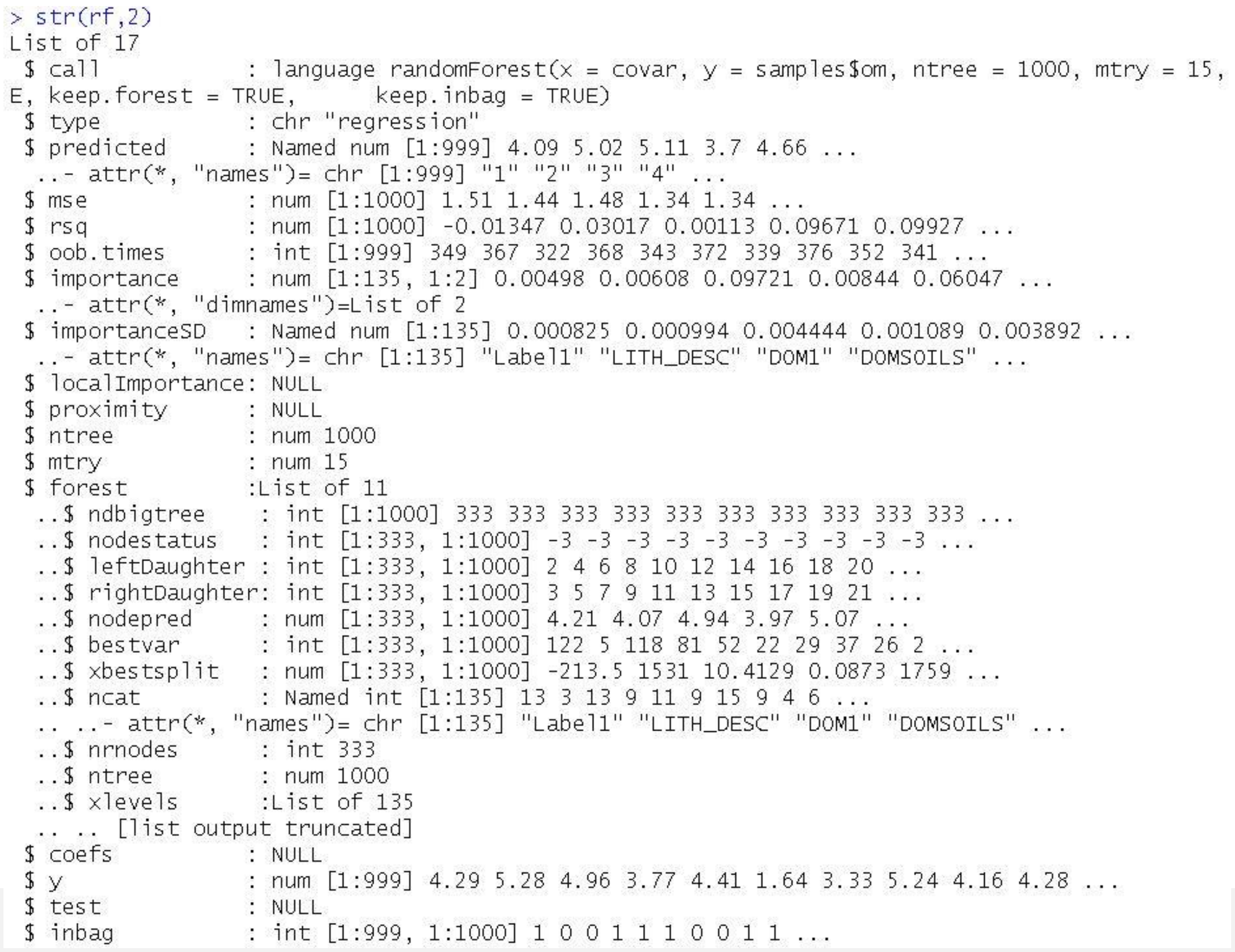
```r
### Random forests modelling ###
library(randomForest)

# create object with target variable
tval <- samples$om

#create object with covariates
covar <- samples[,20:157]

# fit random forests model
rf <- randomForest(
  x = covar,
  y = tval,
  mtry = 15,            # number of randomly selected covariates, default p/3, sqrt(p)
  ntree = 1000,         # number of trees
  nodesize = 10,        # minimum size of terminal nodes
  importance = TRUE,    # assess importance of predictors
  keep.forest = TRUE,   # keep the forest in the output
  keep.inbag = TRUE     # keep track of which samples are "in-bag"
)
```

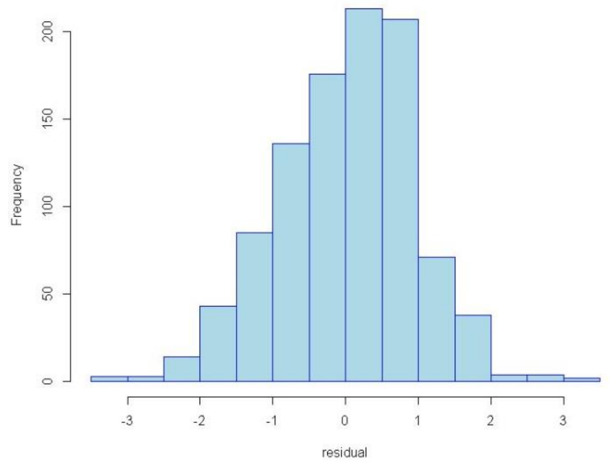
The random forest model in R

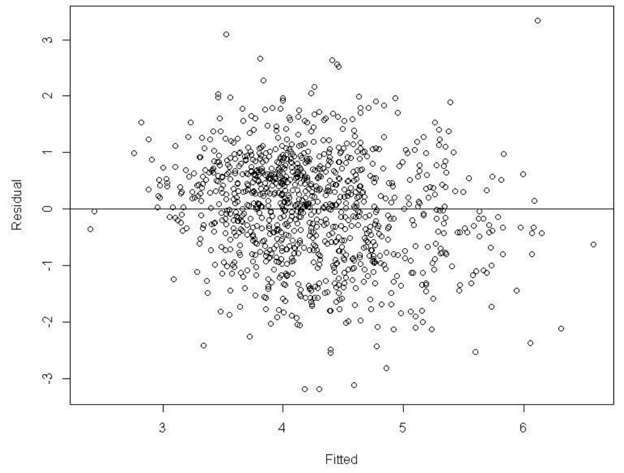


```
> str(rf,2)
List of 17
 $ call           : language randomForest(x = covar, y = samples$om, ntree = 1000, mtry = 15,
E, keep.forest = TRUE,      keep.inbag = TRUE)
 $ type           : chr "regression"
 $ predicted      : Named num [1:999] 4.09 5.02 5.11 3.7 4.66 ...
  ..- attr(*, "names")= chr [1:999] "1" "2" "3" "4" ...
 $ mse            : num [1:1000] 1.51 1.44 1.48 1.34 1.34 ...
 $ rsq            : num [1:1000] -0.01347 0.03017 0.00113 0.09671 0.09927 ...
 $ oob.times      : int [1:999] 349 367 322 368 343 372 339 376 352 341 ...
 $ importance     : num [1:135, 1:2] 0.00498 0.00608 0.09721 0.00844 0.06047 ...
  ..- attr(*, "dimnames")=List of 2
 $ importanceSD   : Named num [1:135] 0.000825 0.000994 0.004444 0.001089 0.003892 ...
  ..- attr(*, "names")= chr [1:135] "Label1" "LITH_DESC" "DOM1" "DOMSOILS" ...
 $ localImportance: NULL
 $ proximity      : NULL
 $ ntree          : num 1000
 $ mtry           : num 15
 $ forest         :List of 11
  ..$ ndbigtree    : int [1:1000] 333 333 333 333 333 333 333 333 333 333 ...
  ..$ nodestatus   : int [1:333, 1:1000] -3 -3 -3 -3 -3 -3 -3 -3 -3 -3 ...
  ..$ leftDaughter : int [1:333, 1:1000] 2 4 6 8 10 12 14 16 18 20 ...
  ..$ rightDaughter: int [1:333, 1:1000] 3 5 7 9 11 13 15 17 19 21 ...
  ..$ nodepred     : num [1:333, 1:1000] 4.21 4.07 4.94 3.97 5.07 ...
  ..$ bestvar      : int [1:333, 1:1000] 122 5 118 81 52 22 29 37 26 2 ...
  ..$ xbestsplit   : num [1:333, 1:1000] -213.5 1531 10.4129 0.0873 1759 ...
  ..$ ncat         : Named int [1:135] 13 3 13 9 11 9 15 9 4 6 ...
  .. ..- attr(*, "names")= chr [1:135] "Label1" "LITH_DESC" "DOM1" "DOMSOILS" ...
  ..$ nrnodes      : int 333
  ..$ ntree        : num 1000
  ..$ xlevels      :List of 135
  .. .. [list output truncated]
 $ coefs          : NULL
 $ y              : num [1:999] 4.29 5.28 4.96 3.77 4.41 1.64 3.33 5.24 4.16 4.28 ...
 $ test           : NULL
 $ inbag          : int [1:999, 1:1000] 1 0 0 1 1 1 0 0 1 1 ...
```

Random forest residuals

- The randomForest function returns predicted values of the input data based on out-of-bag samples.
- Model residuals can be computed: predicted – observed (rf$predicted-rf$y).
- Check assumptions on residuals (prior to geostatistical analysis): normality, constant variance





- Fit variogram, krige residuals, add kriged residuals to RF predictions

Variable importance

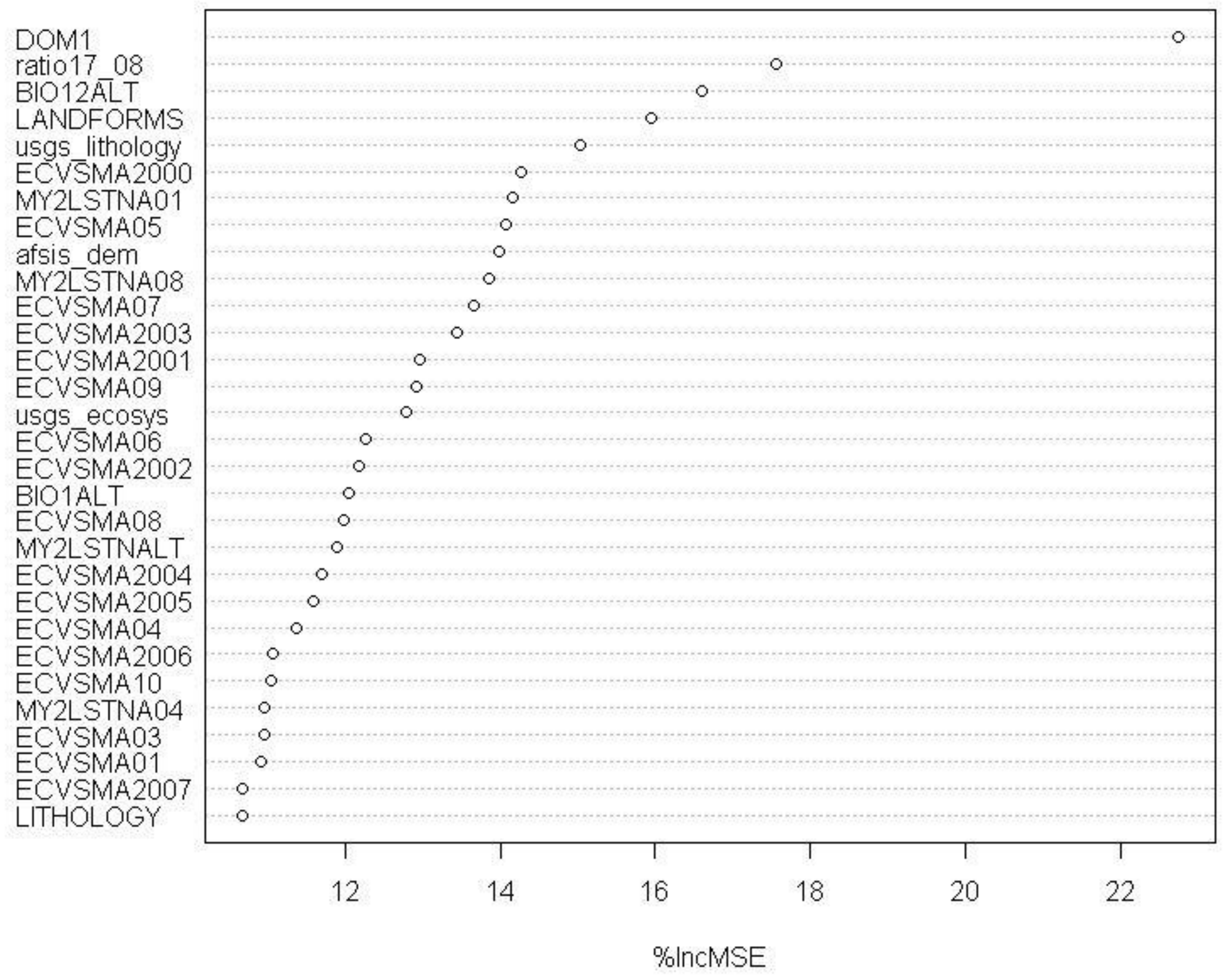
- Ensembles of trees are not easy to interpret: no such thing as an average tree; an individual tree does not tell much.

- Ensemble can reflect the potentially (complex) effect of a variable on the response $\longrightarrow$ assess the relevance of each variable over all trees of the ensemble.

- Variable importance plot: shows how much prediction error increases when the **values** of one predictor **are permuted** (break association with response) while all others are left unchanged.

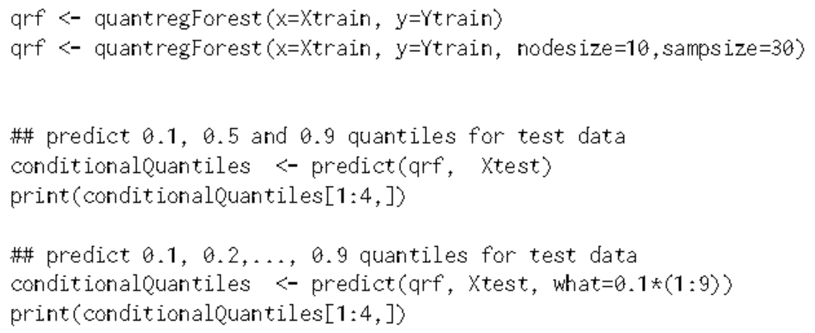
- Permuted variable is used together with other variables to predict the response $\longrightarrow$ prediction accuracy will decrease.

Variable importance plot



Uncertainty assessment

- Uncertainty associated to random forest predictions cannot be easily qualified and is an field of ongoing research and online discussions.
- Methods are computationally intensive (requires much memory)!
- R package **quantregForest**: compute quantiles for predictions.



```
qrf <- quantregForest(x=Xtrain, y=Ytrain)
qrf <- quantregForest(x=Xtrain, y=Ytrain, nodesize=10,sampsize=30)


## predict 0.1, 0.5 and 0.9 quantiles for test data
conditionalQuantiles  <- predict(qrf,  Xtest)
print(conditionalQuantiles[1:4,])

## predict 0.1, 0.2,..., 0.9 quantiles for test data
conditionalQuantiles  <- predict(qrf, Xtest, what=0.1*(1:9))
print(conditionalQuantiles[1:4,])
```

- Pragmatic approach: predict *n* values for each location, compute variance or standard deviation, and from these confidence intervals:

```
pred.rf <- predict(rf, newdata = newdata, predict.all = TRUE)

pred.rfvar <- apply(pred.rf$individual, MARGIN = 1, FUN =var)
```

Optimizing tuning parameters

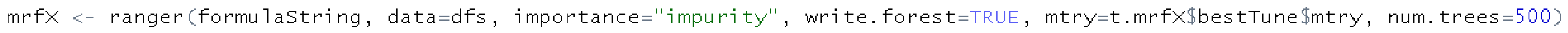
- Instead of using the default one can try to find an optimal value for the **mtry** parameter.
- **train** function of the **caret** package:

```
ctrl <- trainControl(method="repeatedcv", number=3, repeats=1, savePredictions = "final")
rf.tuneGrid <- expand.grid(mtry = seq(4,20,by=2))
t.mrfX <- train(formulaString.lst[[j]], data=dfs, method="rf", trControl=ctrl, tuneGrid=rf.tuneGrid)
t.mrfX$bestTune$mtry
```

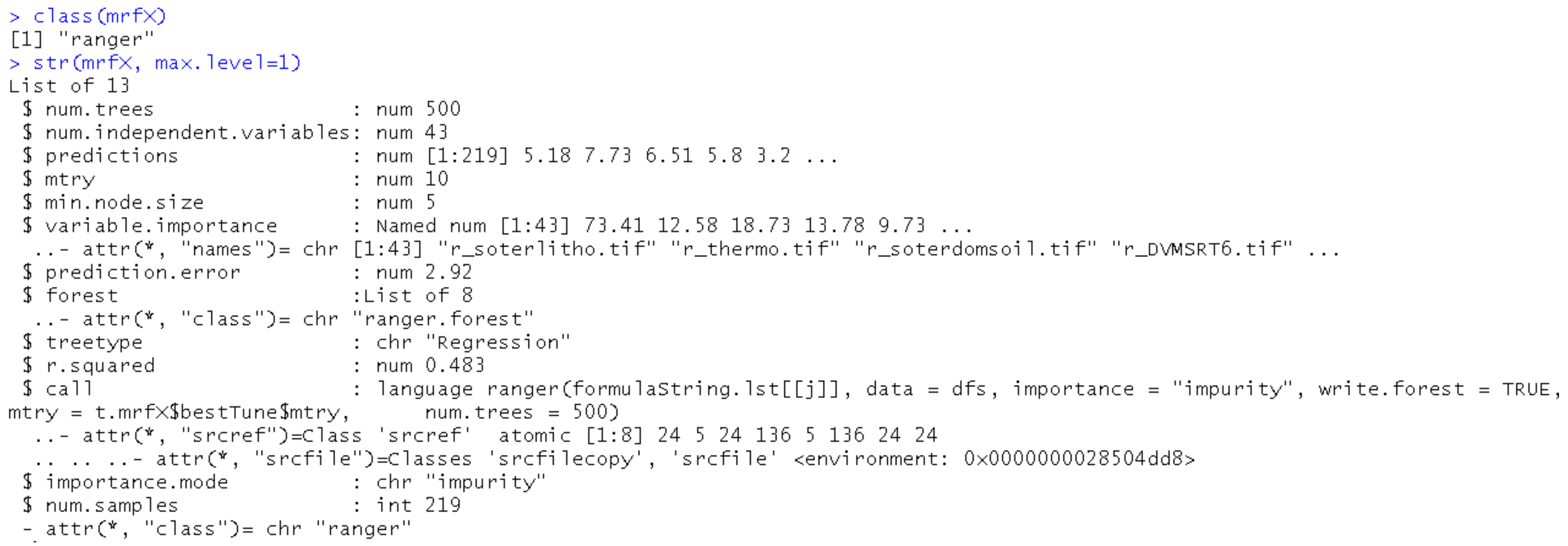
- Offer the optimal **mtry** value to the **randomForest** function
- Try various **ntree** values (e.g. 500, 750, 1000, 1500)

ranger package

- Random forest models can also be fitted with the **ranger** package.
- Faster implementation; allows parallel computing.



```
mrfX <- ranger(formulaString, data=dfs, importance="impurity", write.forest=TRUE, mtry=t.mrfX$bestTune$mtry, num.trees=500)
```



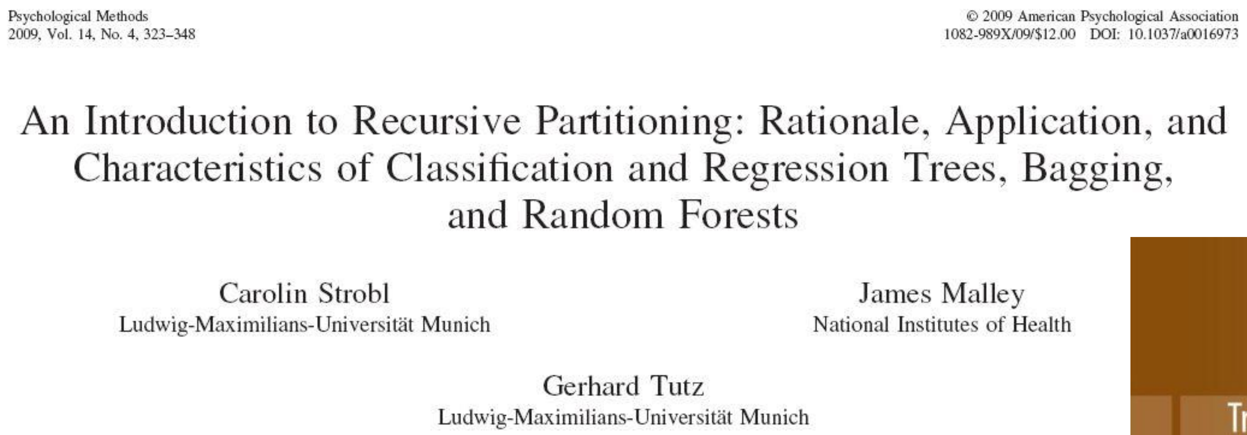
```
> class(mrfX)
[1] "ranger"
> str(mrfX, max.level=1)
List of 13
 $ num.trees                : num 500
 $ num.independent.variables: num 43
 $ predictions              : num [1:219] 5.18 7.73 6.51 5.8 3.2 ...
 $ mtry                     : num 10
 $ min.node.size            : num 5
 $ variable.importance      : Named num [1:43] 73.41 12.58 18.73 13.78 9.73 ...
  ..- attr(*, "names")= chr [1:43] "r_soterlitho.tif" "r_thermo.tif" "r_soterdomsoil.tif" "r_DVMSRT6.tif" ...
 $ prediction.error         : num 2.92
 $ forest                   :List of 8
  ..- attr(*, "class")= chr "ranger.forest"
 $ treetype                 : chr "Regression"
 $ r.squared                : num 0.483
 $ call                     : language ranger(formulaString.lst[[j]], data = dfs, importance = "impurity", write.forest = TRUE,
mtry = t.mrfX$bestTune$mtry,      num.trees = 500)
  ..- attr(*, "srcref")=Class 'srcref'  atomic [1:8] 24 5 24 136 5 136 24 24
  .. .. ..- attr(*, "srcfile")=Classes 'srcfilecopy', 'srcfile' <environment: 0x0000000028504dd8>
 $ importance.mode          : chr "impurity"
 $ num.samples              : int 219
 - attr(*, "class")= chr "ranger"
```

Be aware

- No clear interpretation.
- Prediction uncertainty not easy to quantify (computationally intensive).
- Spatial correlation cannot be accounted for when fitting the model.
- Bias in variable selection (Strobl et al. 2009).
- Stability of the forest depends on ntree, mtry settings.

Recources

- https://www.stat.berkeley.edu/~breiman/RandomForests/cc_home.htm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An Introduction to Recursive Partitioning: Rationale, Application, and Characteristics of Classification and Regression Trees, Bagging, and Random Forests

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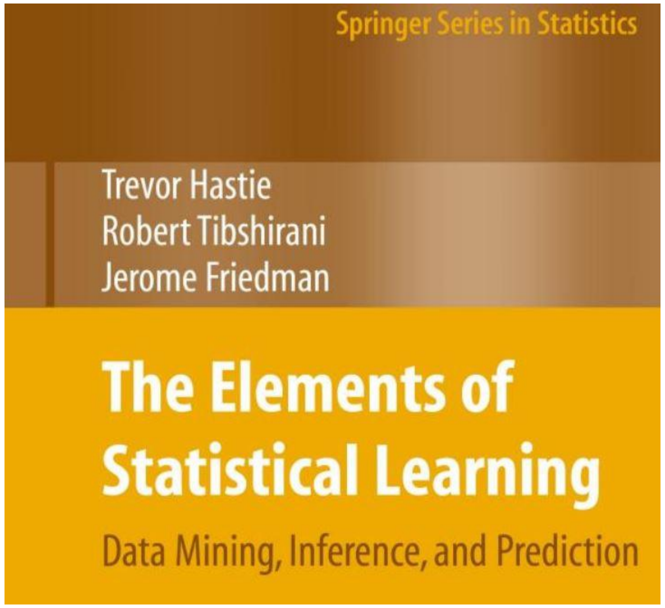
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