Answers to exercises Session 5

Marjolein Fokkema

Exercise 1

Read in data:

```
load("MASQ.Rda")
set.seed(1)
train <- sample(1:nrow(MASQ), size = nrow(MASQ)*.8)
summary(MASQ)
```

```
##  D_DEPDYS       AD               AA              GDD             GDA
##  0:1927   Min.   : 26.00   Min.   :17.00   Min.   :12.00   Min.   :11.0
##  1:1670   1st Qu.: 64.00   1st Qu.:22.00   1st Qu.:20.00   1st Qu.:19.0
##           Median : 77.00   Median :28.00   Median :29.00   Median :24.0
##           Mean   : 75.05   Mean   :32.01   Mean   :30.64   Mean   :25.4
##           3rd Qu.: 88.00   3rd Qu.:39.00   3rd Qu.:40.00   3rd Qu.:31.0
##           Max.   :110.00   Max.   :83.00   Max.   :60.00   Max.   :54.0
##       GDM          leeftijd    geslacht
##  Min.   :15.0   Min.   :17.0   m:1317
##  1st Qu.:31.0   1st Qu.:28.0   v:2280
##  Median :40.0   Median :38.0
##  Mean   :40.6   Mean   :38.8
##  3rd Qu.:50.0   3rd Qu.:48.0
##  Max.   :75.0   Max.   :91.0
```

```
round(cor(MASQ[train, sapply(MASQ, is.numeric)]), digits = 2)
```

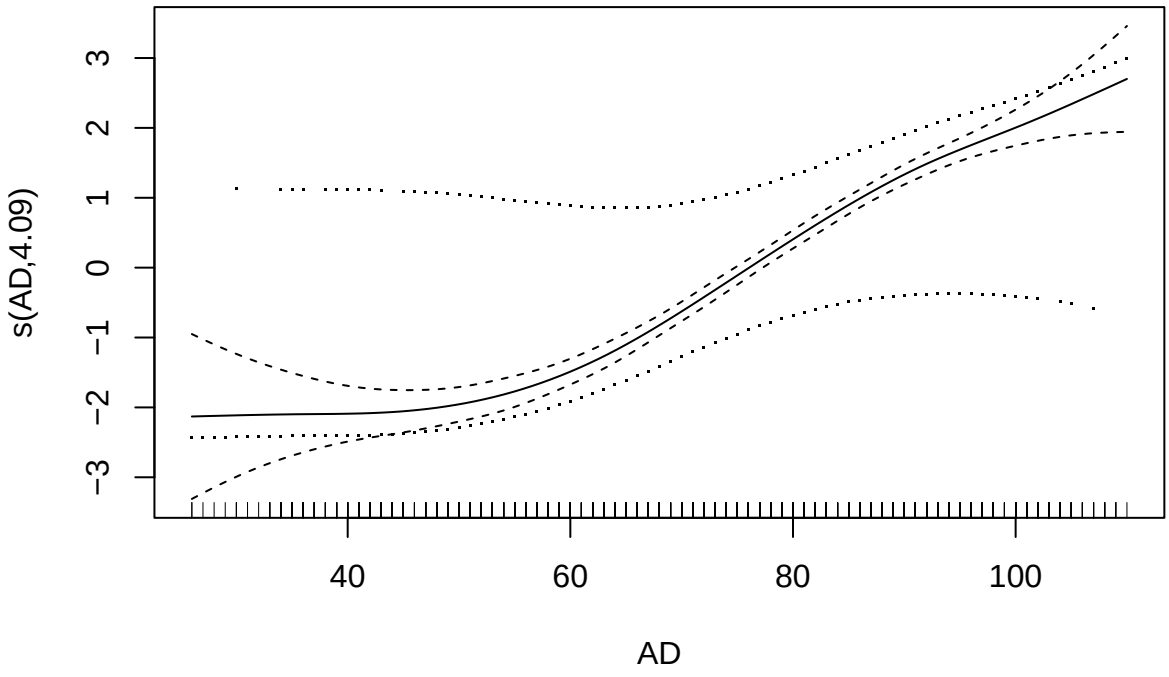
```
##              AD   AA   GDD   GDA   GDM leeftijd
## AD         1.00 0.51  0.79  0.61  0.74     0.01
## AA         0.51 1.00  0.58  0.79  0.70     0.01
## GDD        0.79 0.58  1.00  0.72  0.81    -0.07
## GDA        0.61 0.79  0.72  1.00  0.80    -0.05
## GDM        0.74 0.70  0.81  0.80  1.00    -0.04
## leeftijd 0.01 0.01 -0.07 -0.05 -0.04     1.00
```

Fit a smoothing spline of the `AD` variable to predict `D_DEPDYS`:

```
library("mgcv")
GAM <- gam(D_DEPDYS ~ s(AD, bs = "cr"),
           data = MASQ[train, ], method = "REML", family = "binomial")
summary(GAM)
```

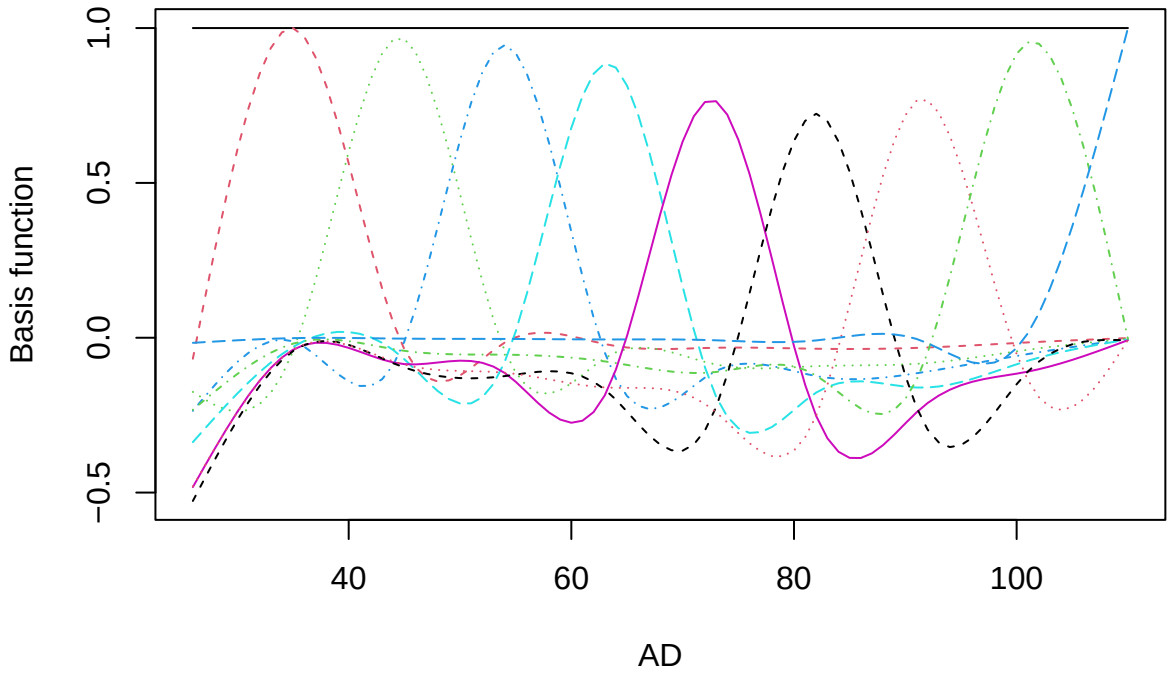
```
##
## Family: binomial
## Link function: logit
##
## Formula:
## D_DEPDYS ~ s(AD, bs = "cr")
##
## Parametric coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept) -0.24089    0.04751   -5.07 3.98e-07 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Approximate significance of smooth terms:
##        edf Ref.df Chi.sq p-value
## s(AD) 4.09  5.041  672.4  <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) =  0.297   Deviance explained = 23.7%
## -REML = 1522.2  Scale est. = 1         n = 2877
```

```
plot(GAM, residuals = TRUE)
```



Inspect the basis functions that were created for `AD`:

```r
mod_mat <- model.matrix(GAM)
matplot(sort(MASQ$AD[train]), mod_mat[order(MASQ$AD[train]), ], type = "l",
        xlab = "AD", ylab = "Basis function")
```



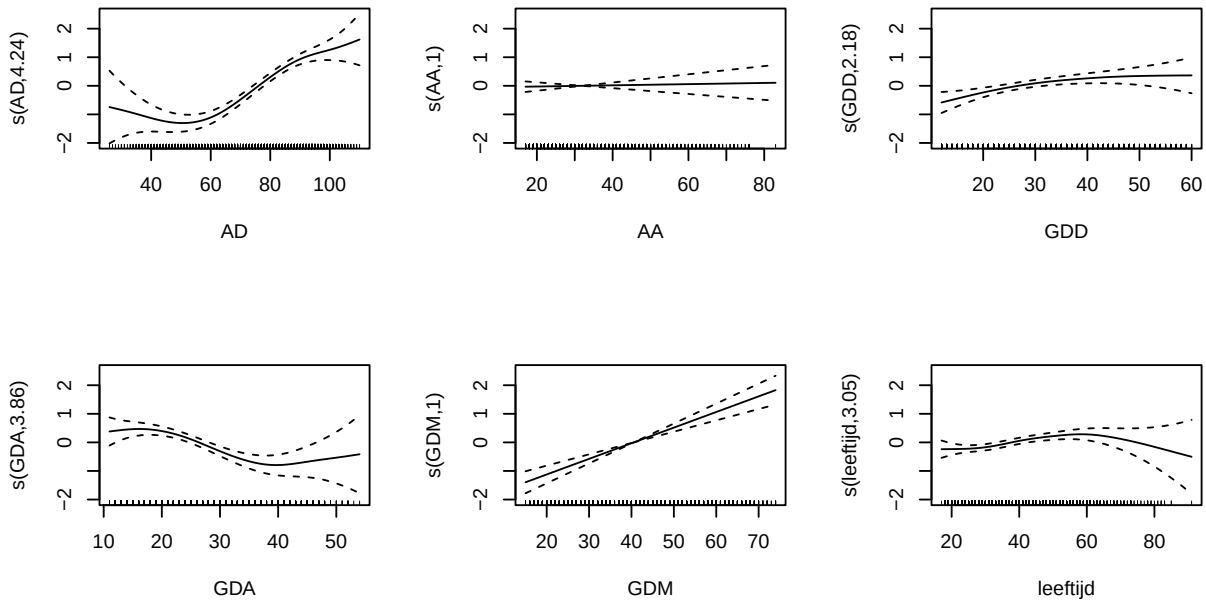
Exercise 2: Multiple predictors

```r
library("mgcv")
GAM <- gam(D_DEPDYS ~ s(AD) + s(AA) + s(GDD) + s(GDA) + s(GDM) + s(leeftijd) + geslacht,
           data = MASQ[train, ], method = "REML", family = "binomial")
summary(GAM)
```

```
##
## Family: binomial
## Link function: logit
##
## Formula:
## D_DEPDYS ~ s(AD) + s(AA) + s(GDD) + s(GDA) + s(GDM) + s(leeftijd) +
##     geslacht
##
## Parametric coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept) -0.33822    0.07755  -4.361 1.29e-05 ***
```

```
## geslachtv    0.13314    0.09517   1.399    0.162
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Approximate significance of smooth terms:
##                edf Ref.df  Chi.sq  p-value
## s(AD)        4.243  5.238 148.910  < 2e-16 ***
## s(AA)        1.001  1.002   0.115  0.73591
## s(GDD)       2.185  2.793  11.185  0.00971 **
## s(GDA)       3.855  4.806  33.279 4.62e-06 ***
## s(GDM)       1.001  1.001  52.723  < 2e-16 ***
## s(leeftijd) 3.050  3.817  17.530  0.00137 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) =  0.331   Deviance explained =   27%
## -REML = 1478.1  Scale est. = 1         n = 2877
```

```r
par(mfrow = c(2, 3))
plot(GAM)
```



We compute the mean squared error and misclassification rate using predicted probabilities, for both training and test observations:

```r
y_train <- as.numeric(MASQ[train, "D_DEPDYS"]) - 1
y_test <- as.numeric(MASQ[-train, "D_DEPDYS"]) - 1

## Training data
GAM_preds_train <- predict(GAM, newdata = MASQ[train, ], type = "response")
mean((y_train - GAM_preds_train)^2) ## Brier score
```

```
## [1] 0.1653101
```

```
tab_train <- prop.table(table(MASQ[train, "D_DEPDYS"], GAM_preds_train > .5)) ## confusion matrix
tab_train
```

```
##
##         FALSE      TRUE
##   0 0.4174487 0.1223497
##   1 0.1160932 0.3441084
```

```
1 - sum(diag(tab_train)) ## MCR
```

```
## [1] 0.2384428
```

```
## Test data
GAM_preds_test <- predict(GAM, newdata = MASQ[-train, ], type = "response")
mean((y_test - GAM_preds_test)^2) ## Brier score
```

```
## [1] 0.1666467
```

```
tab_test <- prop.table(table(MASQ[-train, "D_DEPDYS"], GAM_preds_test > .5)) ## confusion matrix
tab_test
```

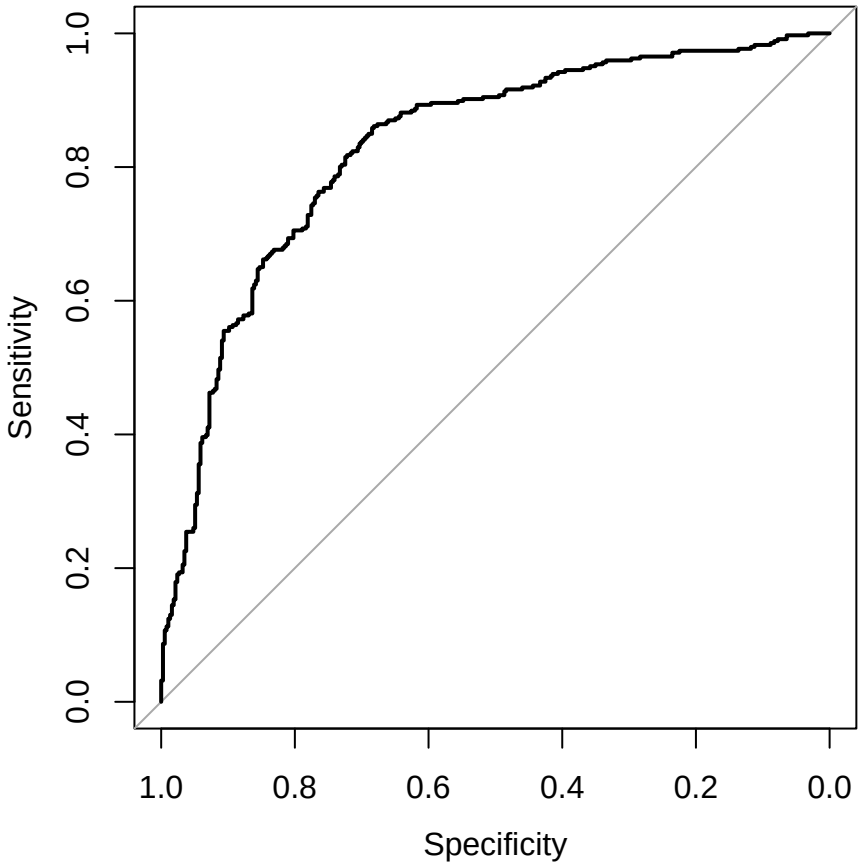
```
##
##         FALSE      TRUE
##   0 0.4027778 0.1166667
##   1 0.1236111 0.3569444
```

```
1 - sum(diag(tab_test)) ## MCR
```

```
## [1] 0.2402778
```

The Brier score and confusion matrices are quite similar between training and test data, indicating little overfitting.

```
## Or, compute ROC curve
library("pROC")
plot(roc(resp = y_test, pred = GAM_preds_test))
```

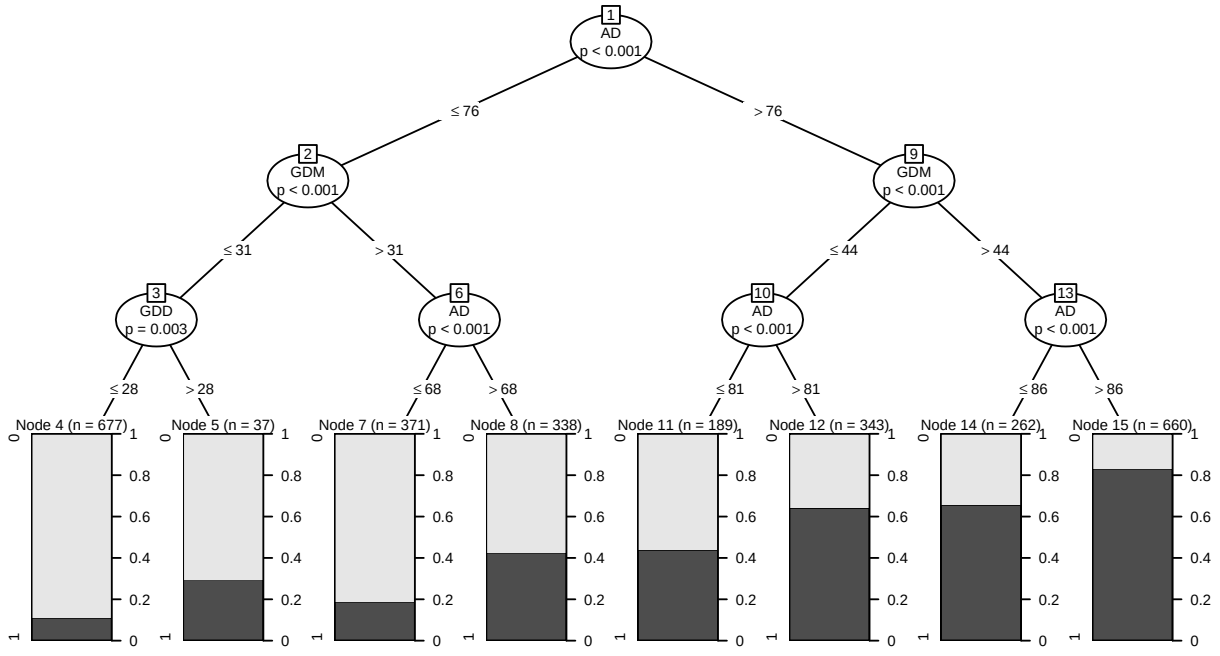



```
auc(resp = y_test, pred = GAM_preds_test)
```

```
## Area under the curve: 0.8295
```

Exercise 4: Fit a conditional inference tree

```
library("partykit")
ct <- ctree(D_DEPDYS ~ . , data = MASQ[train, ])
plot(ct, gp = gpar(cex = .5))
```



The conditional inference tree indicates a positive effect of the AD, GDM and GDD subscales on the probability of having a depressive / dysthymic disorder.

```
## Training data
ct_preds_train <- predict(ct, newdata = MASQ[train, ], type = "prob")[ , 2]
mean((y_train - ct_preds_train)^2) ## Brier score
```

```
## [1] 0.1705674
```

```
tab_train <- prop.table(table(MASQ[train, "D_DEPDYS"], ct_preds_train > .5)) ## confusion matrix
1 - sum(diag(tab_train)) ## MCR
```

```
## [1] 0.2457421
```

```
## Test data
y_test <- as.numeric(MASQ[-train, "D_DEPDYS"]) - 1
ct_preds_test <- predict(ct, newdata = MASQ[-train, ], type = "prob")[ , 2]
mean((y_test - ct_preds_test)^2) ## Brier score
```

```
## [1] 0.1738697
```

```r
tab_test <- prop.table(table(MASQ[-train, "D_DEPDYS"], ct_preds_test > .5)) ## confusion matrix
1 - sum(diag(tab_test)) ## MCR
```

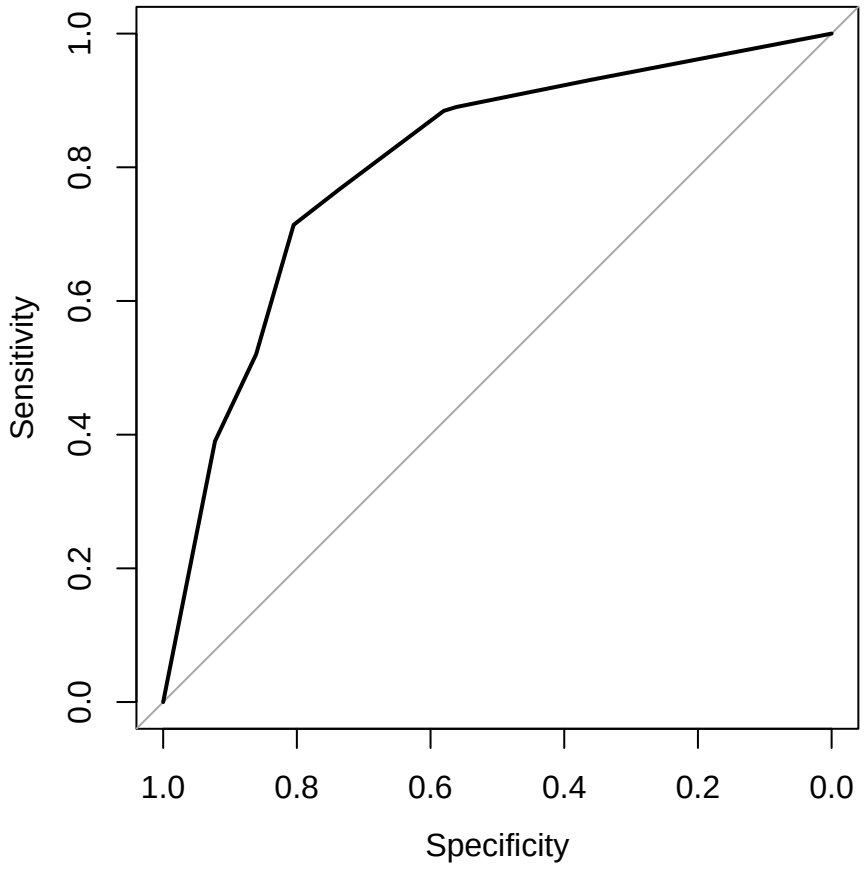
```
## [1] 0.2388889
```

The conditional inference tree provided best predictive accuracy of the single trees.

```r
## AUC on test observations
plot(roc(resp = y_test, pred = ct_preds_test))
```

```
## Setting levels: control = 0, case = 1

## Setting direction: controls < cases
```




```r
auc(resp = y_test, pred = ct_preds_test)
```

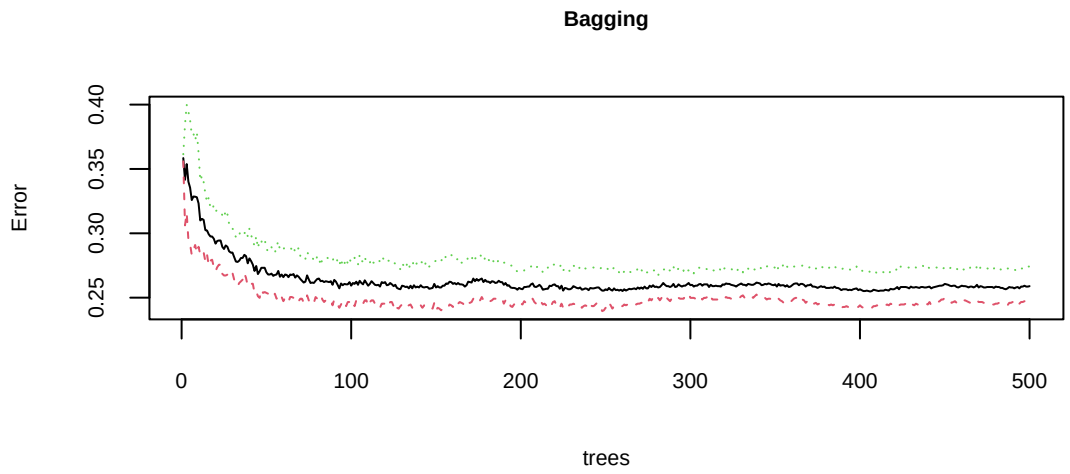
```
## Setting levels: control = 0, case = 1
## Setting direction: controls < cases

## Area under the curve: 0.805
```

Exercise 5: Fit a bagged ensemble and random forest

Fit the ensembles:

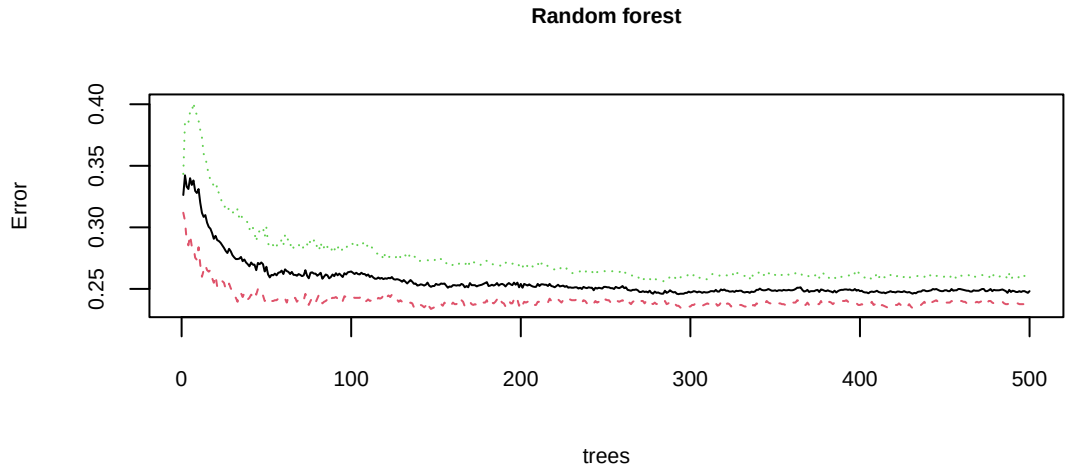
```
library("randomForest")
set.seed(1)
bag.ens <- randomForest(D_DEPDYS ~ AD + AA + GDD + GDA + GDM + leeftijd + geslacht,
                        data = MASQ[train,], importance = TRUE, mtry = 7)
set.seed(1)
rf.ens <- randomForest(D_DEPDYS ~ AD + AA + GDD + GDA + GDM + leeftijd + geslacht,
                       data = MASQ[train,], importance = TRUE, mtry = sqrt(7))
plot(bag.ens, cex.lab = .7, cex.axis = .7, cex.main = .7, main = "Bagging")
```



For these data, the out-of-bag (OOB) error decreases fast with the first 100 trees. After 200-300 trees, the OOB error stabilizes.

Note that for binary classification, three curves are provided: The black curve shows the misclassification error, the green and red curves show the classification error in each of the classes (comparable to sensitivity and specificity).

```
plot(rf.ens, cex.lab = .7, cex.axis = .7, cex.main = .7, main = "Random forest")
```



The OOB error plotted against the number of trees shows a very similar pattern as with the bagged ensemble.

Compute train MCR:

```
tab <- prop.table(table(MASQ[train, "D_DEPDYS"],
                        predict(bag.ens, newdata = MASQ[train,])))
1 - sum(diag(tab))  ## misclassification rate for bagging
```

```
## [1] 0
```

```
tab <- prop.table(table(MASQ[train, "D_DEPDYS"],
                        predict(rf.ens, newdata = MASQ[train,])))
1 - sum(diag(tab)) ## misclassification rate for RF
```

```
## [1] 0
```

Compute test MCR:

```
tab <- prop.table(table(MASQ[-train, "D_DEPDYS"],
predict(bag.ens, newdata = MASQ[-train,])))
1 - sum(diag(tab))  ## misclassification rate for bagging
```

```
## [1] 0.2388889
```

```
tab <- prop.table(table(MASQ[-train, "D_DEPDYS"],
predict(rf.ens, newdata = MASQ[-train,])))
1 - sum(diag(tab)) ## misclassification rate for RF
```

```
## [1] 0.2388889
```

We compute squared error on predicted probabilitites (Brier score) for the training data:

```
predict(bag.ens, newdata = MASQ[train,], type = "prob")[1:10, ]
```

```
##          0     1
## 1017 0.982 0.018
## 679  0.816 0.184
## 2177 0.960 0.040
## 930  0.058 0.942
## 1533 0.788 0.212
## 471  0.998 0.002
## 2347 0.812 0.188
## 270  0.966 0.034
## 1211 0.922 0.078
## 3379 0.878 0.122
```

Note that the predict method returns predicted probabilities for both classes, for objects of class `randomForest`.

Therefore, we selected the second column of the returned probabilities (`[ , 2]`):

```
mean((y_train -
        predict(bag.ens, newdata = MASQ[train,], type = "prob")[ , 2])^2)
```

```
## [1] 0.02466598
```

```
mean((y_train -
        predict(rf.ens, newdata = MASQ[train,], type = "prob")[ , 2])^2)
```

```
## [1] 0.02431729
```

And for the test data:

```
mean((y_test -
        predict(bag.ens, newdata = MASQ[-train,], type = "prob")[ , 2])^2)
```

```
## [1] 0.1765018
```

```
mean((y_test -
        predict(rf.ens, newdata = MASQ[-train,], type = "prob")[ , 2])^2)
```

```
## [1] 0.1723298
```

Test MCRs are identical for the bagged ensemble and random forest. Test SEL is lower for the random forest.

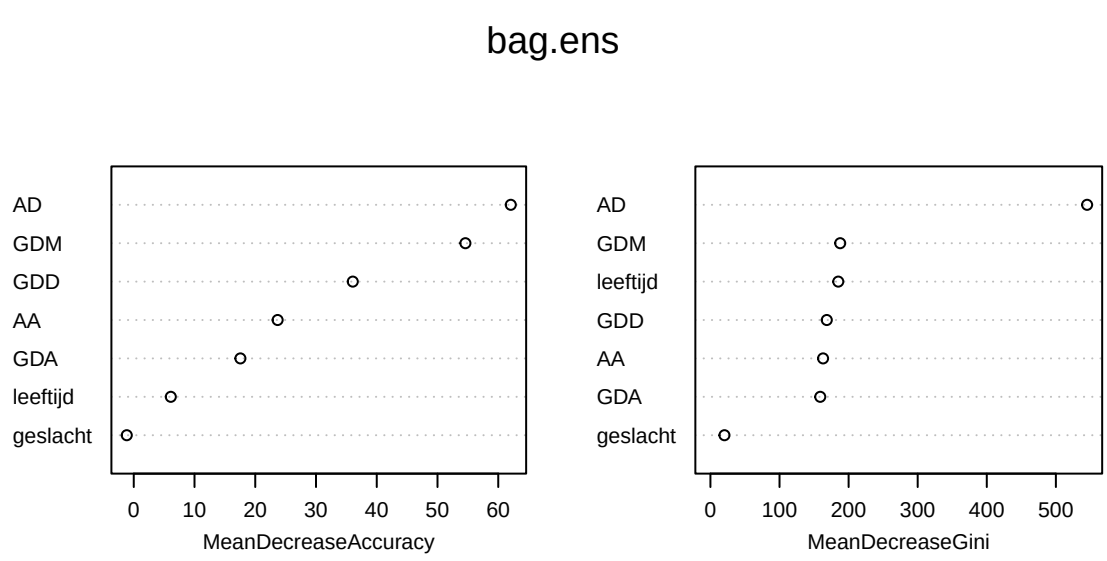
Interpretation

We inspect variable importances:

```r
importance(bag.ens)
```

```
##                  0          1 MeanDecreaseAccuracy MeanDecreaseGini
## AD       26.008074 46.6261372            62.061330        545.20309
## AA       11.210061 19.5952066            23.683674        163.04057
## GDD      24.875687 18.2097877            36.050773        168.41636
## GDA      18.096720  3.1288186            17.552676        158.92755
## GDM      24.393229 39.5161589            54.590675        187.79771
## leeftijd  2.752565  5.6442541             6.098998        185.04514
## geslacht -1.634730 -0.1247933            -1.150591         20.31331
```

```r
varImpPlot(bag.ens, cex = .7, cex.main = .7)
```



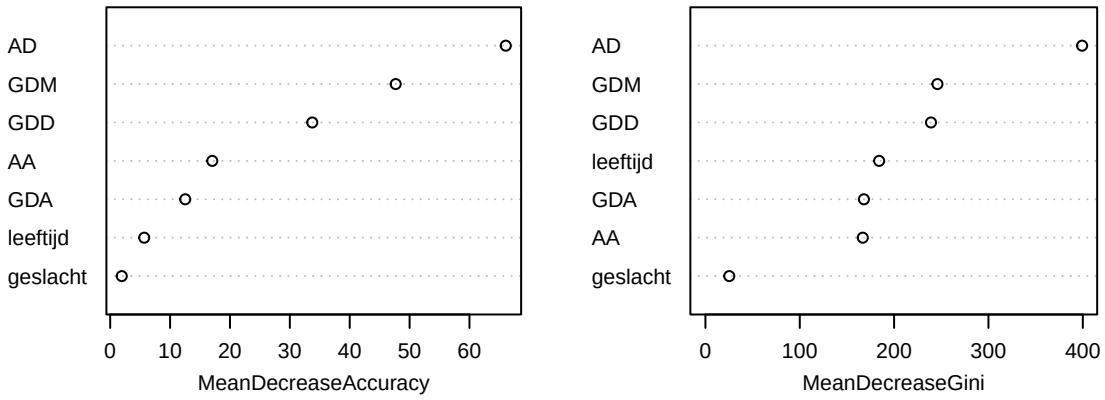
According to the reduction in MSE for the out-of-bag observations (left panel) if the values of each predictor variable are permuted, the AD (anhedonic depression), GDM (general distress mixed), and GDD (general distress depression) are the most important predictors of a depressive disorder diagnosis.

According to the improvement in node purity (i.e., training error; right panel), AD, leeftijd (age) and GDM are the most important predictors of of a depressive disorder diagnosis.

```r
importance(rf.ens)
```

```
##                  0          1 MeanDecreaseAccuracy MeanDecreaseGini
## AD       33.630440 48.266024            66.064052        399.27306
## AA        6.599139 15.579649            17.047234        166.79307
## GDD      22.394085 16.774428            33.745150        239.10990
## GDA      13.584839  1.184124            12.532481        168.00515
## GDM      21.001515 36.662315            47.677333        245.91414
## leeftijd  1.773007  5.834744             5.682049        184.13887
## geslacht  1.344184  1.423987             1.931168         25.26403
```

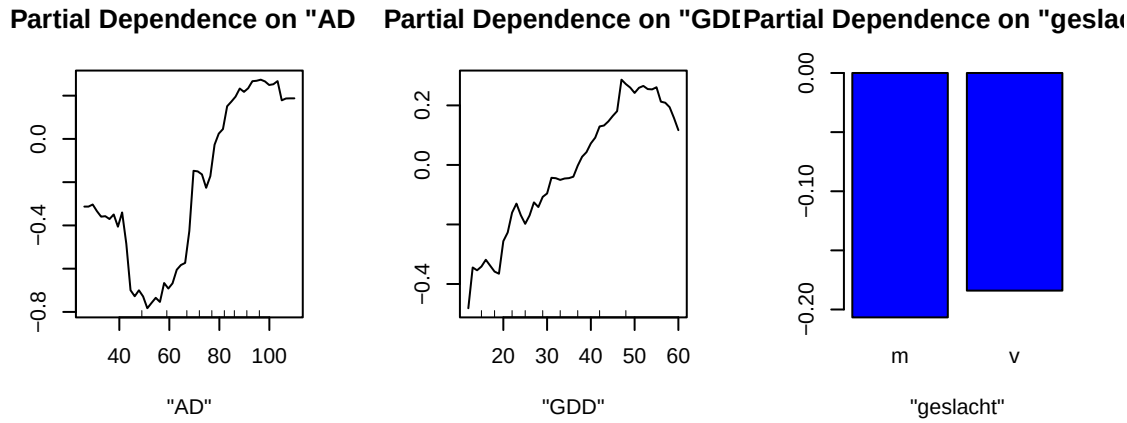
```r
varImpPlot(rf.ens, cex = .7, cex.main = .7)
```



The AD, GDM and GDD scales appear most important in the random forest.

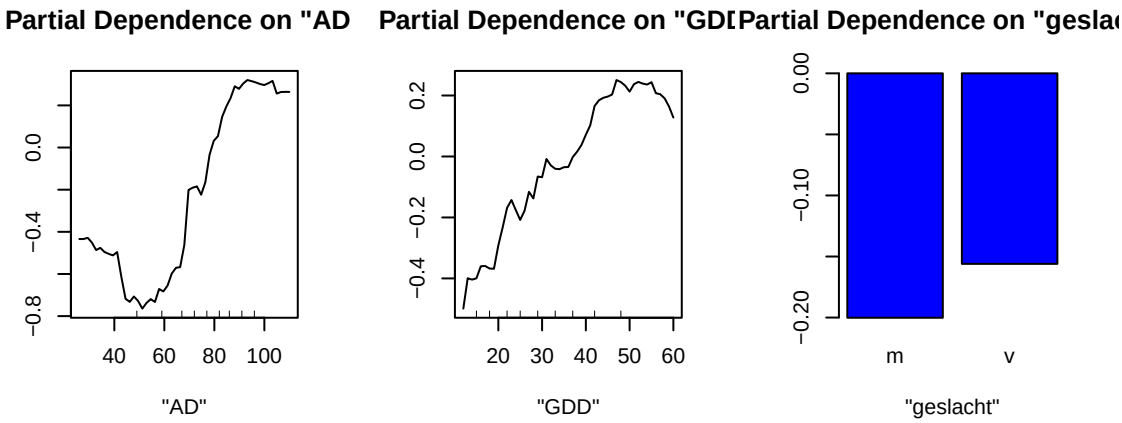
We request partial dependence plots for the bagged ensemble:

```
par(mfrow = c(1, 3))
partialPlot(bag.ens, x.var = "AD", pred.data = MASQ[train,], which.class = "1")
partialPlot(bag.ens, x.var = "GDD", pred.data = MASQ[train,], which.class = "1")
partialPlot(bag.ens, x.var = "geslacht", pred.data = MASQ[train,], which.class = "1")
```



Note that we have to specify the appropriate class label for these plots if we perform classification, otherwise we get partial dependence plots for the effect on the probability of belonging to the first ("0", non-depressed) class.

```
par(mfrow = c(1, 3))
partialPlot(rf.ens, x.var = "AD", pred.data = MASQ[train,], which.class = "1")
partialPlot(rf.ens, x.var = "GDD", pred.data = MASQ[train,], which.class = "1")
partialPlot(rf.ens, x.var = "geslacht", pred.data = MASQ[train,], which.class = "1")
```



Exercise 6: Fit a gradient boosted ensemble

```
library("gbm")
```

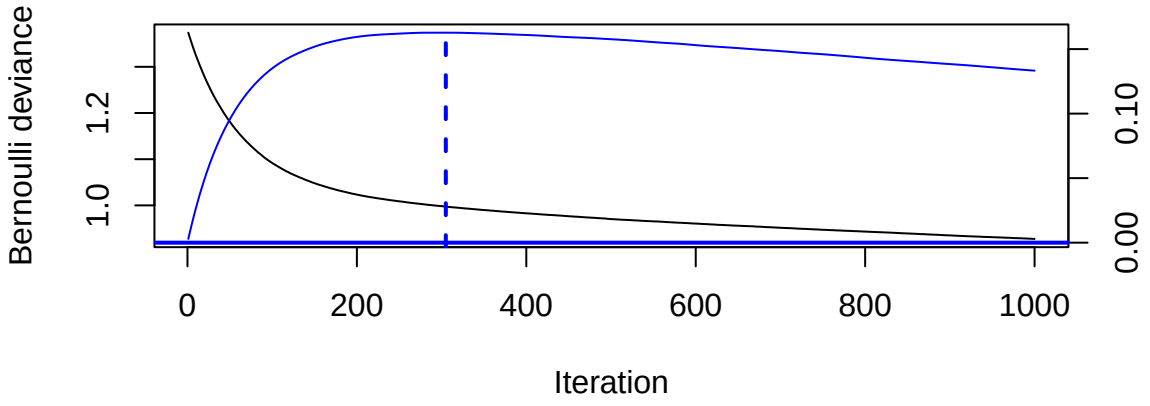
```
## Loaded gbm 2.1.8.1
```

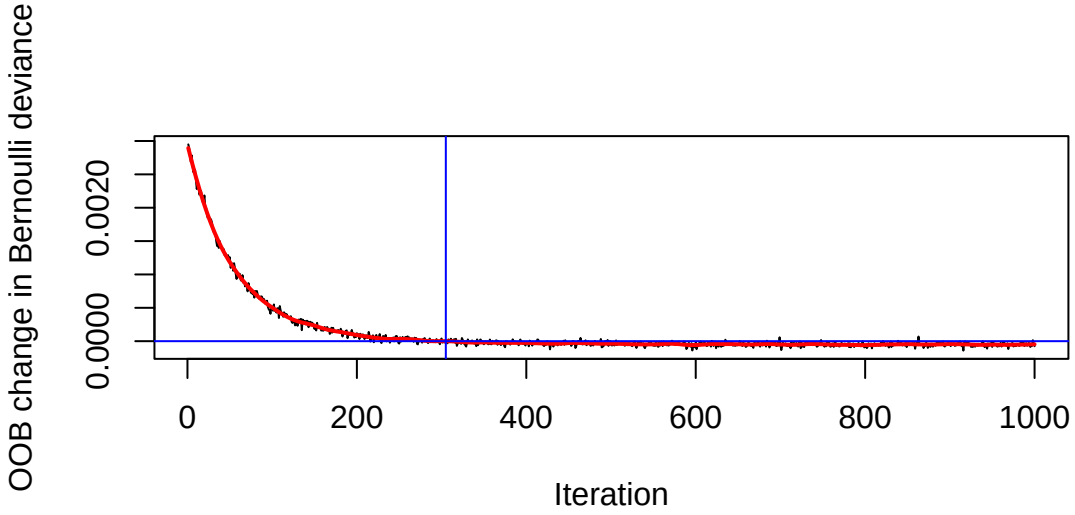
```
set.seed(1)
MASQ$D_DEPDYS <- as.numeric(MASQ$D_DEPDYS) - 1 ## note: gbm wants a numeric response
boost.ens <- gbm(D_DEPDYS ~ ., data = MASQ[train, ], n.trees = 1000,
                 shrinkage = .01, interaction.depth = 4,
                 distribution = "bernoulli")
```

The `n.trees` argument controls the number of generated trees, which defaults to 100. The `bag.fraction` argument controls the fraction of training set observations randomly generated to fit each tree in the ensemble. Tree depth is controlled by argument `interaction.depth`, which defaults to 1 (trees with a single split, i.e., 2 terminal nodes, i.e., main effects only). The learning rate is controlled by the `shrinkage argument`, which defaults to 0.001.

```
gbm.perf(boost.ens, method = "OOB", oobag.curve = TRUE)
```

```
## OOB generally underestimates the optimal number of iterations although predictive performance is reas
```






```
## [1] 305
## attr(,"smoother")
## Call:
## loess(formula = object$oobag.improve ~ x, enp.target = min(max(4,
##     length(x)/10), 50))
##
## Number of Observations: 1000
## Equivalent Number of Parameters: 40
## Residual Standard Error: 3.229e-05
```

The black curve in the first plot represents training error, which decreases as a function of the number of iterations (fitted trees). The blue curve represents the estimated cumulative improvement in the deviance as estimated based on OOB observations (we requested this through specifying `oobag.curve = TRUE`).

In the first plot, the vertical blue dotted line indicates at which iteration the OOB error starts increasing (instead of decreasing). In the second plot, we see that this is where the OOB change in deviance becomes

negative instead of positive. Thus, this appears the optimal number of iterations (according to the OOB deviance).

We also obtained a warning that OOB generally underestimates the number of required iterations, so the initial value of 1000 might not be bad, also because the second plot indicates no big risk of overfitting (i.e., although the OOB change in deviance becomes negative, but it remains very close to 0).

```
## Train performance
gbm_preds_train <- predict(boost.ens, newdata = MASQ[train,], type = "response")
```

```
## Using 1000 trees...
```

```
tab_train <- prop.table(table(true = y_train, predicted = gbm_preds_train > .5))
tab_train
```

```
##     predicted
## true     FALSE      TRUE
##    0 0.4209246 0.1188738
##    1 0.1021898 0.3580118
```

```
1 - sum(diag(tab_train)) ## misclassification rate
```

```
## [1] 0.2210636
```

```
mean((y_train - gbm_preds_train)^2) ## brier score
```

```
## [1] 0.1502326
```

```
## Test performance
gbm_preds_test <- predict(boost.ens, newdata = MASQ[-train,], type = "response")
```

```
## Using 1000 trees...
```

```
tab_test <- prop.table(table(true = y_test, predicted = gbm_preds_test > .5))
tab_test
```

```
##     predicted
## true     FALSE      TRUE
##    0 0.4000000 0.1194444
##    1 0.1180556 0.3625000
```

```
1 - sum(diag(tab_test)) ## misclassification rate
```

```
## [1] 0.2375
```

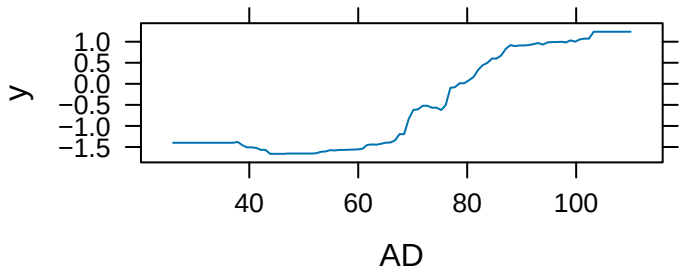
```
mean((y_test - gbm_preds_test)^2) ## brier score
```

```
## [1] 0.1675675
```

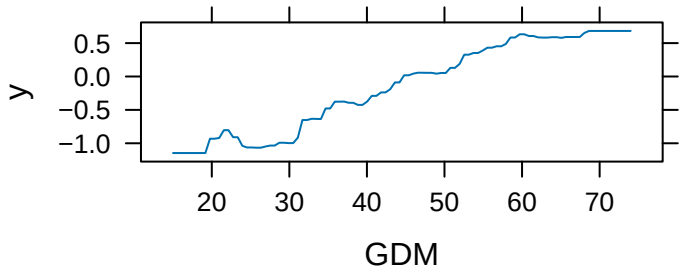
This seems to be the lowest test error we obtained thus far. We will further improve by tuning the parameters in the next exercise.

Interpretation

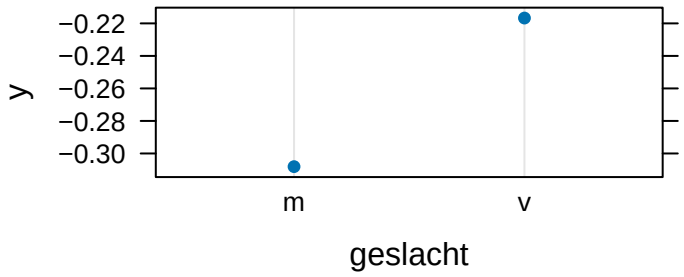
```
plot(boost.ens, i.var = "AD")
```




```
plot(boost.ens, i.var = "GDM")
```



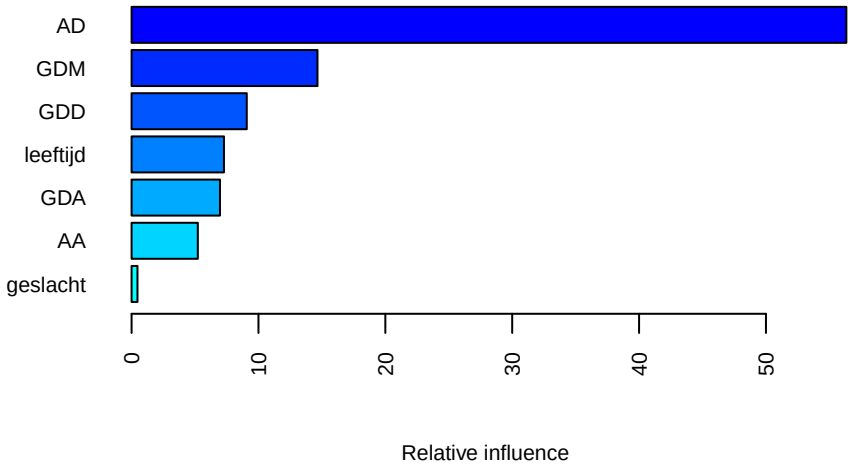

```
plot(boost.ens, i.var = "geslacht")
```



The partial dependence plot suggest that the higher the AD and GDM scale scores, the higher the probability of having depression or dysthymia. Men appear to have a slightly lower probability of having a diagnosis, compared to women.

We request a summary of the model in order to obtain variable importances:

```
summary(boost.ens, cex.lab = .7, cex.axis = .7, cex.sub = .7, cex = .7, las = 2)
```



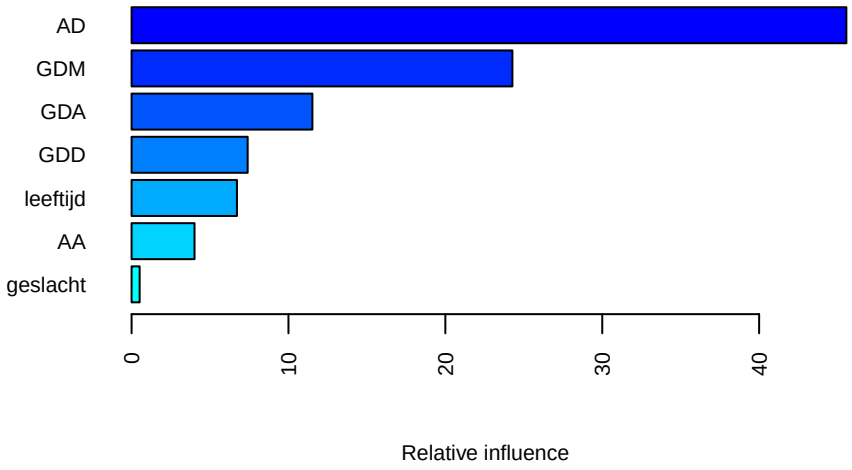

```
##                var    rel.inf
## AD              AD 56.3372131
## GDM            GDM 14.6522092
## GDD            GDD  9.0783275
## leeftijd leeftijd  7.2809713
## GDA            GDA  6.9666723
## AA              AA  5.2209153
## geslacht geslacht  0.4636913
```

Through the various `cex` arguments, we set the size of text and plotting symbols. Through the `las` argument, we specify the orientation of the axis labels (see `?par` for more explanation).

Like with the bagged and random forest ensembles, again we find that the AD variable is the strongest predictor of depressive disorder, followed by GDM and GDD.

Function `gbm()` return importances based on training error, by default (see `?summary.gbm`). We can obtain permutation importances (but note: these are computed using both in-bag and OOB observations, see also `?summary.gbm`) through specifying the method argument:

```
summary(boost.ens, cex.lab = .7, cex.axis = .7, cex.sub = .7, cex = .7,
        method = permutation.test.gbm, las = 2)
```




```
##        var    rel.inf
## 1       AD 45.5601747
## 2      GDM 24.2750184
## 3      GDA 11.5252439
## 4      GDD  7.3987442
## 5 leeftijd  6.7159431
## 6       AA  4.0113324
## 7 geslacht  0.5135434
```

Tuning parameters

```
library("caret")
grid <- expand.grid(shrinkage = c(.1, .01, .001),
                    n.trees = c(10, 100, 1000),
                    interaction.depth = 1:4,
                    n.minobsinnode = 10)
head(grid, 6)
```

```
##   shrinkage n.trees interaction.depth n.minobsinnode
## 1     0.100      10                 1             10
## 2     0.010      10                 1             10
## 3     0.001      10                 1             10
## 4     0.100     100                 1             10
## 5     0.010     100                 1             10
## 6     0.001     100                 1             10
```

```
tail(grid, 6)
```

```
##    shrinkage n.trees interaction.depth n.minobsinnode
```

```
## 31      0.100      100                 4             10
## 32      0.010      100                 4             10
## 33      0.001      100                 4             10
## 34      0.100     1000                 4             10
## 35      0.010     1000                 4             10
## 36      0.001     1000                 4             10
```

Above, we created a grid of tuning parameters that predictive accuracy will be assessed over. As the `train()` function from package caret employs sub sampling to assess performance of the models, we have to set the random seed to allow for future replication of our results. Note that running the following code fits repeatedly fits boosted models for each set of parameter values, so it will take some time to run.

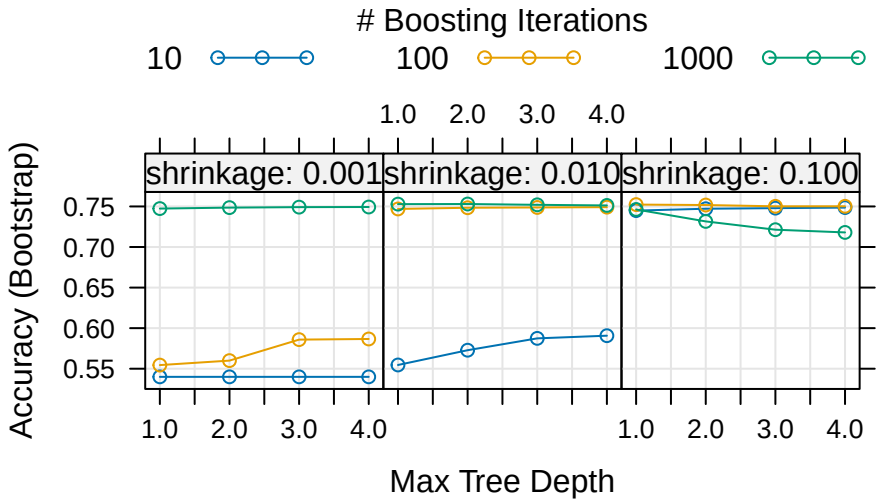
Note that `train()` requires a factor as the response for classification task, (unlike function `gbm()`), so I set the response to be a factor:

```
traindat <- MASQ[train, ]
traindat$D_DEPDYS <- as.factor(traindat$D_DEPDYS)
set.seed(42)
gbmFit <- train(D_DEPDYS ~ . , data = traindat, tuneGrid = grid,
                distribution = "bernoulli", method = "gbm", verbose = FALSE)
```

Check out `?train` and `?trainControl` (which explains the arguments passed to argument `trControl`) to see what we did with this code. The default of bootstrap sampling with 25 repeats was used, (see `method` and `number` arguments of in `?trainControl`). Note that these predictive accuracies are estimated on test observations (i.e., 'OOB' observations).

We plot the results:

```
plot(gbmFit)
```



Note that the highest accuracies are close to what we have obtained with the models we fitted before. The plot suggests that with higher values of shrinkage, we need less boosting iterations, which is as expected. Note that several combinations of parameter settings appear to yield similar accuracy.

Increasing tree depth to values > 1 seems not to make much different, only seems beneficial when there are less trees, suggesting mostly main effects of the predictor variables.

The best accuracy is obtained with:

```
gbmFit$bestTune
```

```
##    n.trees interaction.depth shrinkage n.minobsinnode
## 18    1000                 2      0.01             10
```

These optimal settings differ, but not by much, from our original parameter settings.

We refit the ensemble using the parameter values that can be expected to optimize predictive accuracy:

```
set.seed(42)
boost.ens2 <- gbm(D_DEPDYS ~ ., data = MASQ[-train,], n.trees = 1000,
                  shrinkage = .01, interaction.depth = 2,
                  distribution = "bernoulli")

## Train performance
gbm2_preds_train <- predict(boost.ens2, newdata = MASQ[train,], type = "response")
```

```
## Using 1000 trees...
```

```
tab_train <- prop.table(table(true = y_train, predicted = gbm2_preds_train > .5))
1 - sum(diag(tab_train))
```

```
## [1] 0.2502607
```

```
mean((y_train - gbm2_preds_train)^2)
```

```
## [1] 0.1759091
```

```
## Test performance
gbm2_preds_test <- predict(boost.ens2, newdata = MASQ[-train,], type = "response")
```

```
## Using 1000 trees...
```

```
tab_test <- prop.table(table(true = y_test, predicted = gbm2_preds_test > .5))
tab_test
```

```
##     predicted
## true      FALSE       TRUE
##    0 0.42361111 0.09583333
##    1 0.09166667 0.38888889
```

```
1 - sum(diag(tab_test))
```

```
## [1] 0.1875
```

```r
mean((y_test - gbm2_preds_test)^2)
```

```
## [1] 0.135182
```

Both MCR and SEL improved compared to the earlier boosted ensemble. The boosted ensemble with tuned parameters also outperformed the random forest and bagged ensemble fitted to these data previously. All fitted tree ensembles require all variables for making a prediction (because all variables have non-zero importances).

The CART tree requires only the AD scale for prediction. The ctree requires only the variables AD and GDD, and in some cases also GDD for prediction. They thus require substantially less information for prediction, but at a cost to predictive accuracy.