Solution 1: Bagging

- Let's first think about the expectation – what is the stochastic part we integrate over? Since the base learner and ensemble structure is fixed for given data, the only thing random is the bootstrap sample we use as training data for the m-th tree, given that the total available training data originate from the data-generating process $\mathbb{P}_{xy}$, so we could write $\mathbb{E}_{\mathcal{D}_{\text{train}}^{[m]} \mid \mathcal{D}_{\text{train}} \sim \mathbb{P}_{xy}}$ (for ease of notation, we'll omit the subscripts of the expectation from now on).
- Next, consider the quantity we are supposed to compare to another quantity: $\mathbb{E}\left(\left(y - b^{[m]}(\mathbf{x})\right)^2\right)$. This looks already a lot like the $\mathbb{E}(Z^2)$ part of the LOTV.
- Since the expectation is linear, it is often worthwhile to decompose expressions of expectation and isolate the stochastic parts. Here, the only thing that changes w.r.t. $\mathcal{D}_{\text{train}}^{[m]}$ is the base learner models $b^{[m]}(\mathbf{x})$:

$$\begin{aligned}\mathbb{E}\left(\left(y - b^{[m]}(\mathbf{x})\right)^2\right) &= \mathbb{E}\left(y^2 - 2yb^{[m]}(\mathbf{x}) + \left(b^{[m]}(\mathbf{x})\right)^2\right) \\ &= y^2 - 2y\mathbb{E}\left(b^{[m]}(\mathbf{x})\right) + \mathbb{E}\left(\left(b^{[m]}(\mathbf{x})\right)^2\right),\end{aligned}$$

- Now it's time to realize two things. First: we want to arrive at $\left(y - \mathbb{E}\left(b^{[m]}(\mathbf{x})\right)\right)^2$ in order to be able to use the $(\mathbb{E}(Z))^2$ part of the LOTV. Second: the RHS of the above expression looks almost like a binomial formula – we just need to move the square in the last term:

$$y^2 - 2y\mathbb{E}\left(b^{[m]}(\mathbf{x})\right) + \left(\mathbb{E}\left(b^{[m]}(\mathbf{x})\right)\right)^2 = \left(y - \mathbb{E}\left(b^{[m]}(\mathbf{x})\right)\right)^2$$

- Combine the two parts using the LOTV:

$$\mathbb{E}\left(\left(y - b^{[m]}(\mathbf{x})\right)^2\right) \geq \left(y - \mathbb{E}\left(b^{[m]}(\mathbf{x})\right)\right)^2.$$

- The last missing step is to show that $\mathbb{E}\left(b^{[m]}(\mathbf{x})\right) = f^{[M]}(\mathbf{x})$. To compute the expectation for this discrete random variable (we have a finite ensemble), we sum over all possible realizations, weighted by their probability of occurence. This can be further simplified given that all of the M bootstrap samples were drawn with equal probability:

$$\begin{aligned}\mathbb{E}\left(b^{[m]}(\mathbf{x})\right) &= \sum_{m=1}^{M} b^{[m]}(\mathbf{x}) p\left(\mathcal{D}_{\text{train}}^{[m]}\right) \\ &= \sum_{m=1}^{M} b^{[m]}(\mathbf{x}) \cdot \frac{1}{M} \\ &= \frac{1}{M} \sum_{m=1}^{M} b^{[m]}(\mathbf{x}),\end{aligned}$$

  which is precisely the ensemble prediction $f^{[M]}(\mathbf{x})$.
- Putting everything together, we get

$$\mathbb{E}\left(\left(y - b^{[m]}(\mathbf{x})\right)^2\right) \geq \left(y - \left(f^{[M]}(\mathbf{x})\right)\right)^2,$$

  showing that the expected quadratic loss over individual base learner predictions is at least as large as the expected loss of the ensemble prediction.

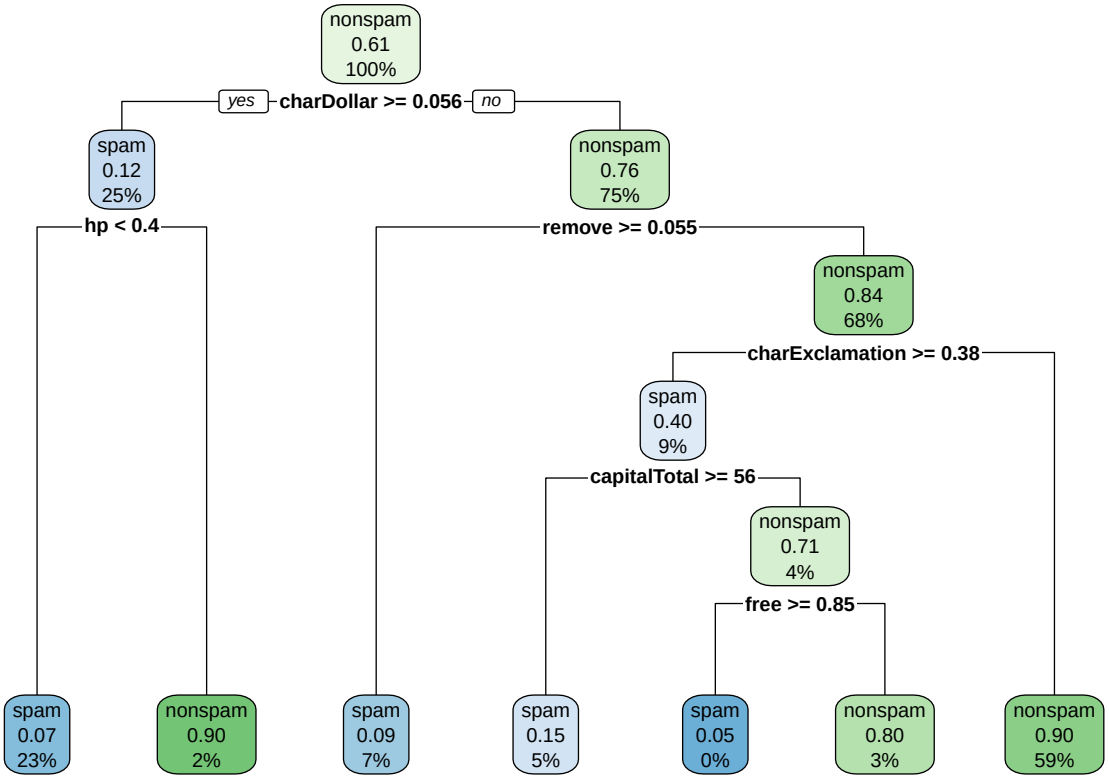
Solution 2: Classifying `spam`

a) The `spam` data is a binary classification task where the aim is to classify an e-mail as spam or non-spam.

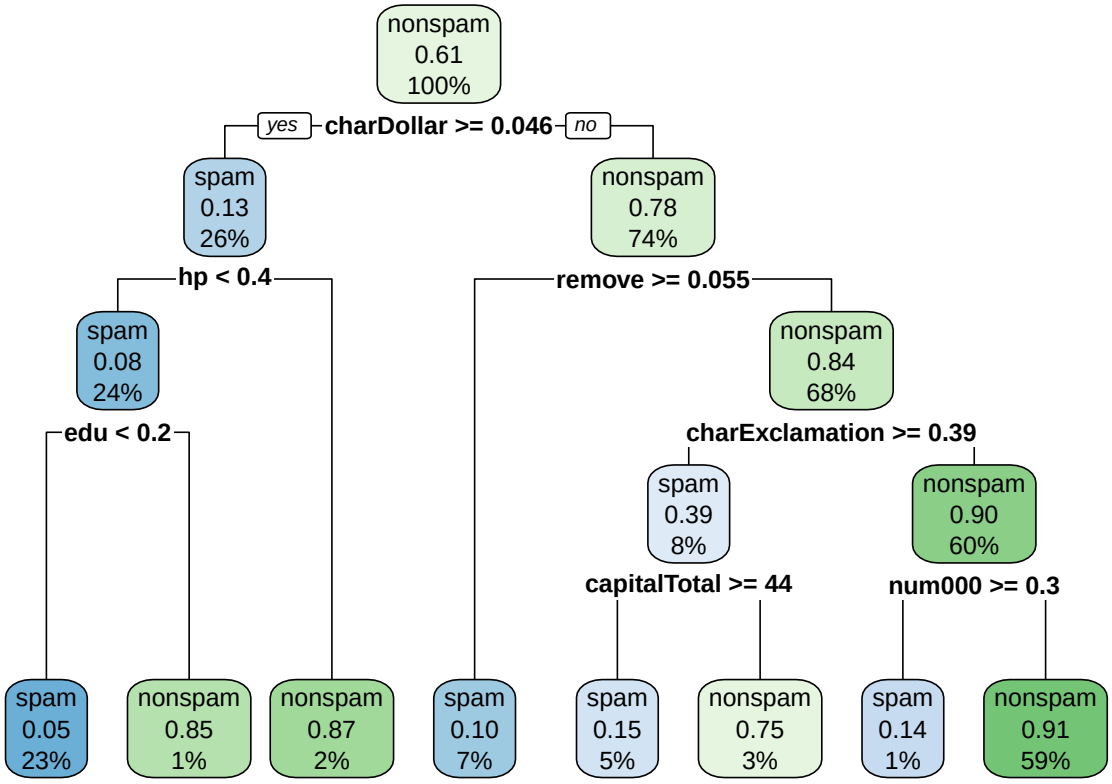
```
library(mlr3)
tsk("spam")

## <TaskClassif:spam> (4601 x 58): HP Spam Detection
## * Target: type
## * Properties: twoclass
## * Features (57):
##   - dbl (57): address, addresses, all, business, capitalAve,
##     capitalLong, capitalTotal, charDollar, charExclamation, charHash,
##     charRoundbracket, charSemicolon, charSquarebracket, conference,
##     credit, cs, data, direct, edu, email, font, free, george, hp, hpl,
##     internet, lab, labs, mail, make, meeting, money, num000, num1999,
##     num3d, num415, num650, num85, num857, order, original, our, over,
##     parts, people, pm, project, re, receive, remove, report, table,
##     technology, telnet, will, you, your
```

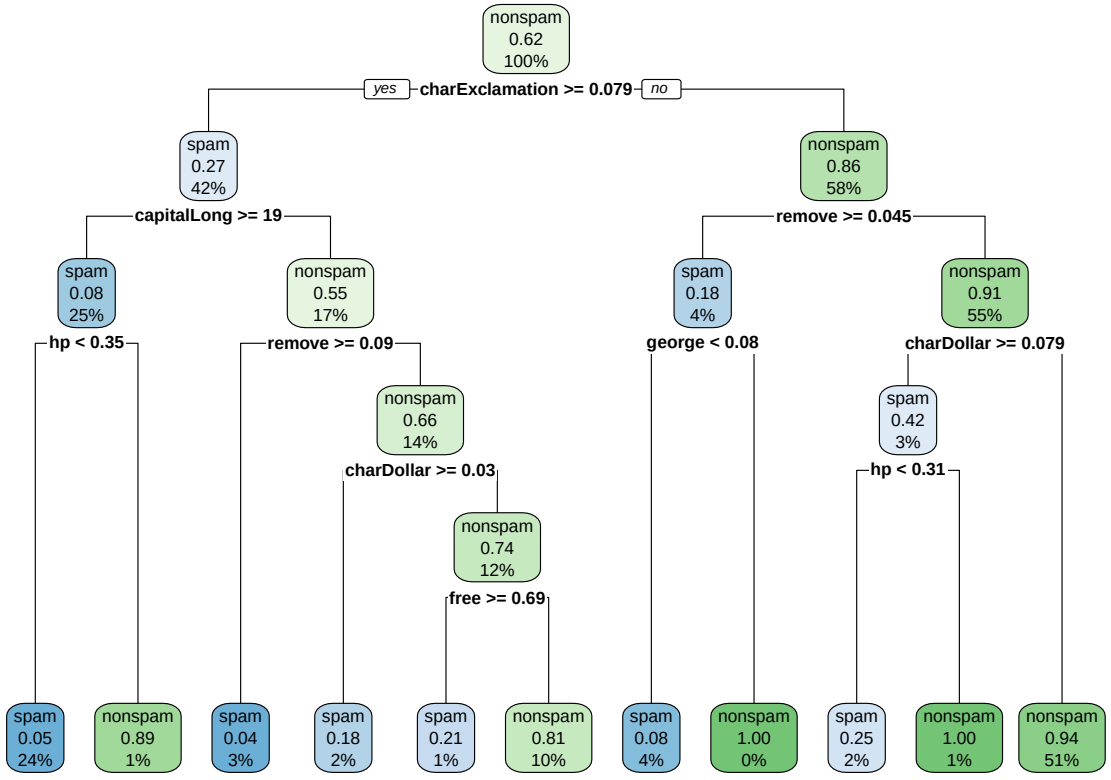
b)

```
library(rpart.plot)
## Loading required package: rpart

task_spam <- tsk("spam")

learner <- lrn("classif.rpart")
learner$train(task_spam)

set.seed(123)
rpart.plot(learner$model, roundint = FALSE)
```




```
set.seed(456)
subset_1 <- sample.int(task_spam$nrow, size = 0.6 * task_spam$nrow)
set.seed(789)
subset_2 <- sample.int(task_spam$nrow, size = 0.6 * task_spam$nrow)

for (i in list(subset_1, subset_2)) {
  learner$train(task_spam, row_ids = i)
  rpart.plot(learner$model, roundint = FALSE)
}
```





Observation: trees trained on different samples differ considerably in their structure, regarding split variables as well as thresholds (recall, though, that the split candidates are a further source of randomness).

c) i) This is actually quite easy when we recall that the exponential function at an arbitrary input x can be characterized via

$$e^x = \lim_{n\to\infty} \left(1 + \frac{x}{n}\right)^n,$$

which already resembles the limit expression we are looking for. Setting x to -1 yields:

$$\lim_{n\to\infty} \left(1 - \frac{1}{n}\right)^n = e^{-1} = \frac{1}{e}.$$

ii)
```
library(mlr3learners)

learner <- lrn("classif.ranger", "oob.error" = TRUE)
learner$train(tsk("spam"))
learner$model$prediction.error

## [1] 0.04542491
```

d) Variable importance in general measures the contributions of features to a model. One way of computing the variable importance of the j-th variable is based on permuting it for the OOB observations and calculating the mean increase in OOB error this permutation entails.

In order to determine the with the biggest influence on prediction quality, we can choose the k variables with the highest importance score, e.g., for $k = 5$:

```
library(mlr3filters)

learner <- lrn("classif.ranger", importance = "permutation", "oob.error" = TRUE)
filter <- flt("importance", learner = learner)
filter$calculate(tsk("spam"))
head(as.data.table(filter), 5)

##            feature      score
## 1:     capitalLong 0.04523183
## 2:              hp 0.04099699
## 3: charExclamation 0.04018370
## 4:          remove 0.03975776
## 5:      capitalAve 0.03412908
```

Solution 3: Proximities

a) Using the `treeInfo()` output, we can follow the path of each sample through each tree.

The following table prints for each observation (rows) their terminal nodes as assigned by trees 1-3. For example, consider observation 1 in tree 1 (first cell): the observation has `phenols` > 1.94, putting it in node 2 (`rightChild` of node 0), from there in node 6 (because it has `alcohol` > 13.04).

```
# end node each observation is placed in across trees
end_nodes

##    tree_1 tree_2 tree_3
## 1:      6      6      6
## 2:      6      5      5
## 3:      6      6      6
```

b) For the proximities, we consider each pair of observations and compute the relative frequency of trees assigning them to the same terminal node.

- Observations 1 and 2: only tree 1 assigns them to the same node, so the proximity is $\frac{1}{3}$.
- Observations 1 and 3: all trees assign them to the same node, so the proximity is 1.
- Observations 2 and 3: only tree 1 assigns them to the same node, so the proximity is $\frac{1}{3}$.

c) We can put this information into a similarity matrix (as such matrices become large quite quickly for more data, it is common to store only the lower diagonal – the rest is non-informative/redundant):

```
library(proxy)
compute_prox <- function(i, j) sum(i == j) / length(i)
round(proxy::dist(end_nodes, method = compute_prox), 2L)

##      1    2
## 2 0.33
## 3 1.00 0.33
```