Introduction to Machine Learning

Working Group "Computational Statistics" – Bernd Bischl et al.

Code demo for resampling

Self made Cross Validation

We want to assess the performance of our model, i.e., try to estimate its generalization error. Why is it a good idea to use cross-validation (CV)?

Let's write our very own CV function for a k-NN learner to experiment with....

```r
library(mlr3)
library(mlr3learners)
library(mlbench)

set.seed(13)
spiral <- as.data.frame(mlbench.spirals(n = 500, sd = 0.1))

# Cross validation for kNN
# inputs:
#   data a data set to use
#   target name of the column in <data>to classify
#   folds number of CV folds
#   k neighborhood size for kNN
# returns vector of test set errors for the different folds
knn_cv <- function(data, target, folds, k) {
  cv_errors <- as.numeric(folds)

  indices <- c(
    sample(x = seq(1, nrow(data), by = 1), size = nrow(data), replace = FALSE),
    rep(NA, (folds - nrow(data) %% folds) %% folds)
  )

  # index matrix for folds
  index_mat <- matrix(data = indices, byrow = FALSE, nrow = folds)

  for (i in 1:folds) {
    # data
    test_data <- data[na.omit(index_mat[i, ]), ]
    train_data <- data[-na.omit(index_mat[i, ]), ]
    task <- TaskClassif$new(
      id = "spirals_train",
      backend = train_data, target = target
    )
    # model
    learner <- lrn("classif.kknn", k = k)
    # train on training set
    learner$train(task = task)
    # evaluate on test data
    cv_errors[i] <- learner$predict_newdata(test_data)$score()
  }

  cv_errors
}

result <- knn_cv(data = spiral, target = "classes", folds = 11, k = 4)
```

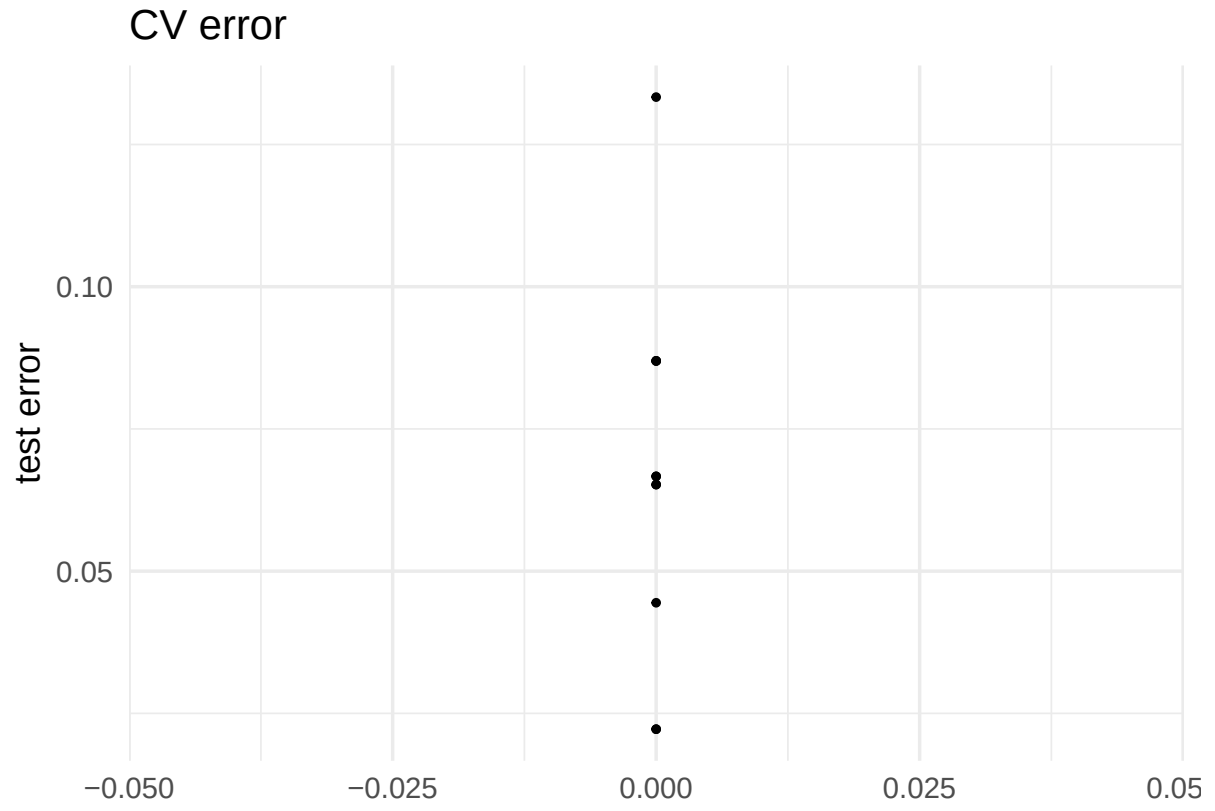
```
result
```

```
##  [1] 0.0652 0.0870 0.0652 0.0870 0.0870 0.0667 0.1333 0.0444
##  [9] 0.0667 0.0222 0.0222
```

```
mean(result)
```

```
## [1] 0.0679
```

```
p <- ggplot(data = as.data.frame(result), aes(y = result)) +
  geom_point(x = 0) +
  ggtitle(label = "CV error") +
  xlab("") + ylab("test error") + xlim(c(0, 0))
p
```

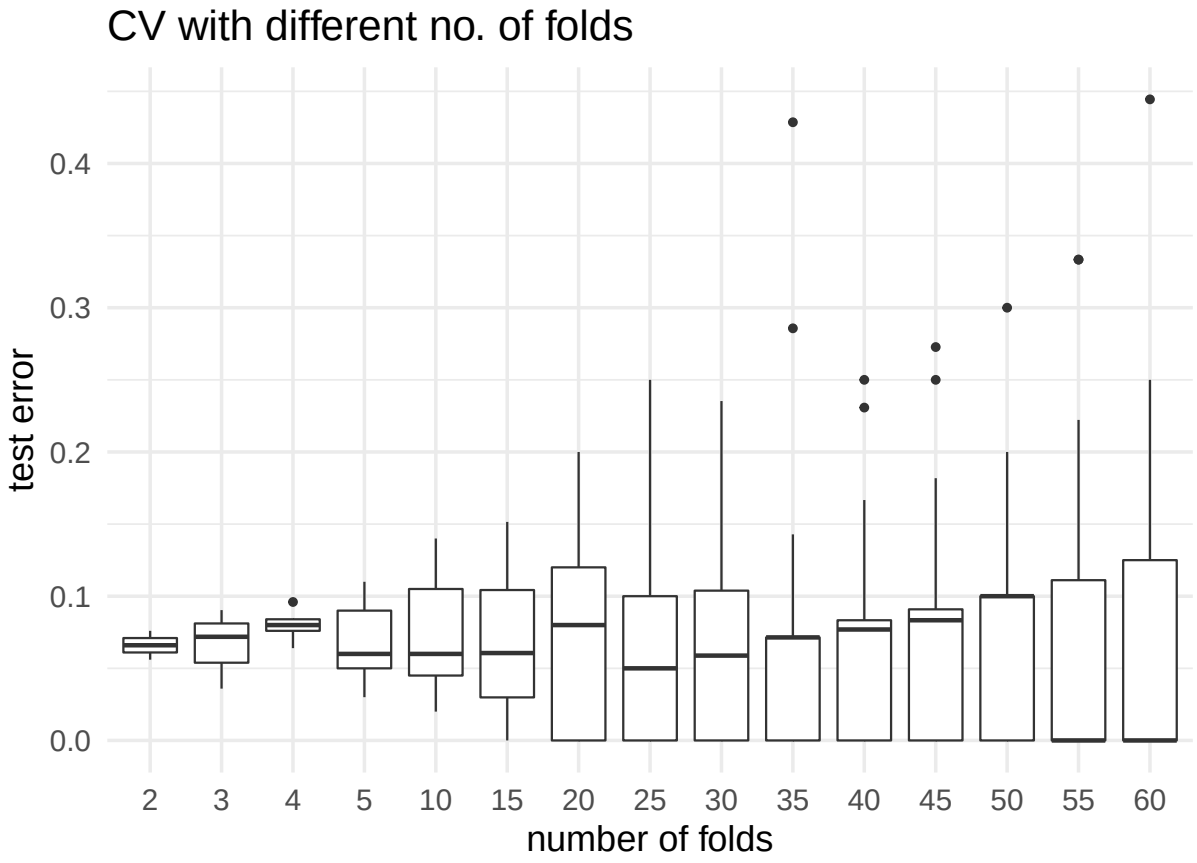


So what happens if we increase the number of folds?

```
# run CV with 2, 3, 4, 5, 10, 15, ...., 60 folds and record the test set errors.
cv_results <- lapply(
  X = c(2, 3, 4, 5 * (1:12)),
  FUN = function(folds) {
    data.frame(
      folds = as.character(folds),
      cv_errors = knn_cv(
        data = spiral, target = "classes",
```

```
        folds = folds, k = 4
      )
    )
  }
)
cv_data <- do.call(rbind, cv_results)


cv_plot <-
  ggplot(cv_data, aes(x = folds, y = cv_errors)) + geom_boxplot() +
  ggtitle(label = "CV with different no. of folds") +
  xlab("number of folds") + ylab("test error")
cv_plot
```



The more we increase the number of folds, the larger each training set becomes. Hence the *pessimistic bias* for the estimated model performance becomes smaller.
But since the test sets also become smaller, the *variance* of the resulting performance estimate increases. In addition, with a higher number of folds, the computation time increases. (Think about that: by how much? is the increase linear in the number of folds? why or why not?)

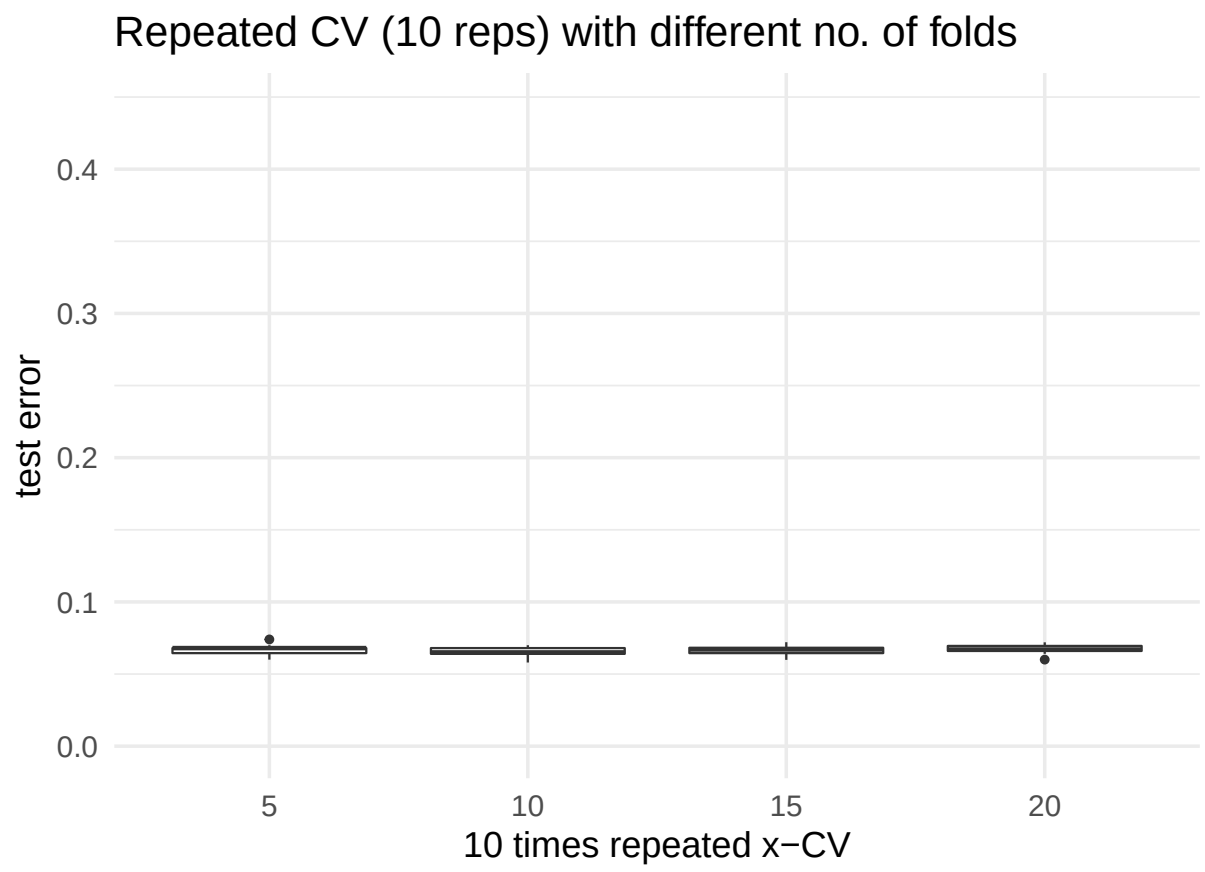
Can we get better results with a smaller amount of computation? Let's see what happens if we do repeated CV and collect only their means:

```
# do reps = 10 repetitions each of 5, 10, 15, 20-fold CV
rep_cv_results <- lapply(
  X = c(5, 10, 15, 20),
```

```
  FUN = function(folds, reps = 10) {
    mean_cv_errors <- replicate(
      reps,
      mean(knn_cv(
        data = spiral, target = "classes",
        folds = folds, k = 4
      ))
    )
    data.frame(
      folds = as.character(folds),
      mean_cv_errors = mean_cv_errors
    )
  }
)

rep_cv_data <- do.call(rbind, rep_cv_results)

ggplot(rep_cv_data, aes(x = folds, y = mean_cv_errors)) +
  geom_boxplot() +
  xlab("10 times repeated x-CV") + ylab("test error") +
  ggtitle(label = "Repeated CV (10 reps) with different no. of folds") +
  ylim(range(cv_data$cv_errors))
```



We see that our estimation results stabilize.

mlr3's CV implementation

```
set.seed(1337)
task <- TaskClassif$new(
  id = "spirals_task",
  backend = spiral, target = "classes"
)
rdesc_cv <- rsmp("repeated_cv", folds = 10, repeats = 10)

mlr_cv <- resample(
  resampling = rdesc_cv, learner = lrn("classif.kknn", k = 4),
  task = task
)
```

```
## INFO  [10:24:51.024] Applying learner 'classif.kknn' on task 'spirals_task' (iter 1/100)
## INFO  [10:24:51.095] Applying learner 'classif.kknn' on task 'spirals_task' (iter 2/100)
## INFO  [10:24:51.148] Applying learner 'classif.kknn' on task 'spirals_task' (iter 3/100)
## INFO  [10:24:51.173] Applying learner 'classif.kknn' on task 'spirals_task' (iter 4/100)
## INFO  [10:24:51.199] Applying learner 'classif.kknn' on task 'spirals_task' (iter 5/100)
## INFO  [10:24:51.224] Applying learner 'classif.kknn' on task 'spirals_task' (iter 6/100)
## INFO  [10:24:51.250] Applying learner 'classif.kknn' on task 'spirals_task' (iter 7/100)
## INFO  [10:24:51.275] Applying learner 'classif.kknn' on task 'spirals_task' (iter 8/100)
## INFO  [10:24:51.301] Applying learner 'classif.kknn' on task 'spirals_task' (iter 9/100)
## INFO  [10:24:51.326] Applying learner 'classif.kknn' on task 'spirals_task' (iter 10/100)
## INFO  [10:24:51.366] Applying learner 'classif.kknn' on task 'spirals_task' (iter 11/100)
## INFO  [10:24:51.393] Applying learner 'classif.kknn' on task 'spirals_task' (iter 12/100)
## INFO  [10:24:51.417] Applying learner 'classif.kknn' on task 'spirals_task' (iter 13/100)
## INFO  [10:24:51.440] Applying learner 'classif.kknn' on task 'spirals_task' (iter 14/100)
## INFO  [10:24:51.462] Applying learner 'classif.kknn' on task 'spirals_task' (iter 15/100)
## INFO  [10:24:51.485] Applying learner 'classif.kknn' on task 'spirals_task' (iter 16/100)
## INFO  [10:24:51.507] Applying learner 'classif.kknn' on task 'spirals_task' (iter 17/100)
## INFO  [10:24:51.529] Applying learner 'classif.kknn' on task 'spirals_task' (iter 18/100)
## INFO  [10:24:51.552] Applying learner 'classif.kknn' on task 'spirals_task' (iter 19/100)
## INFO  [10:24:51.575] Applying learner 'classif.kknn' on task 'spirals_task' (iter 20/100)
## INFO  [10:24:51.597] Applying learner 'classif.kknn' on task 'spirals_task' (iter 21/100)
## INFO  [10:24:51.620] Applying learner 'classif.kknn' on task 'spirals_task' (iter 22/100)
## INFO  [10:24:51.643] Applying learner 'classif.kknn' on task 'spirals_task' (iter 23/100)
## INFO  [10:24:51.666] Applying learner 'classif.kknn' on task 'spirals_task' (iter 24/100)
## INFO  [10:24:51.688] Applying learner 'classif.kknn' on task 'spirals_task' (iter 25/100)
## INFO  [10:24:51.711] Applying learner 'classif.kknn' on task 'spirals_task' (iter 26/100)
## INFO  [10:24:51.734] Applying learner 'classif.kknn' on task 'spirals_task' (iter 27/100)
## INFO  [10:24:51.757] Applying learner 'classif.kknn' on task 'spirals_task' (iter 28/100)
## INFO  [10:24:51.780] Applying learner 'classif.kknn' on task 'spirals_task' (iter 29/100)
## INFO  [10:24:51.802] Applying learner 'classif.kknn' on task 'spirals_task' (iter 30/100)
## INFO  [10:24:51.824] Applying learner 'classif.kknn' on task 'spirals_task' (iter 31/100)
## INFO  [10:24:51.859] Applying learner 'classif.kknn' on task 'spirals_task' (iter 32/100)
## INFO  [10:24:51.890] Applying learner 'classif.kknn' on task 'spirals_task' (iter 33/100)
## INFO  [10:24:51.918] Applying learner 'classif.kknn' on task 'spirals_task' (iter 34/100)
## INFO  [10:24:51.945] Applying learner 'classif.kknn' on task 'spirals_task' (iter 35/100)
## INFO  [10:24:51.972] Applying learner 'classif.kknn' on task 'spirals_task' (iter 36/100)
## INFO  [10:24:51.998] Applying learner 'classif.kknn' on task 'spirals_task' (iter 37/100)
## INFO  [10:24:52.020] Applying learner 'classif.kknn' on task 'spirals_task' (iter 38/100)
## INFO  [10:24:52.043] Applying learner 'classif.kknn' on task 'spirals_task' (iter 39/100)
```

```
## INFO  [10:24:52.065] Applying learner 'classif.kknn' on task 'spirals_task' (iter 40/100)
## INFO  [10:24:52.087] Applying learner 'classif.kknn' on task 'spirals_task' (iter 41/100)
## INFO  [10:24:52.110] Applying learner 'classif.kknn' on task 'spirals_task' (iter 42/100)
## INFO  [10:24:52.132] Applying learner 'classif.kknn' on task 'spirals_task' (iter 43/100)
## INFO  [10:24:52.155] Applying learner 'classif.kknn' on task 'spirals_task' (iter 44/100)
## INFO  [10:24:52.177] Applying learner 'classif.kknn' on task 'spirals_task' (iter 45/100)
## INFO  [10:24:52.200] Applying learner 'classif.kknn' on task 'spirals_task' (iter 46/100)
## INFO  [10:24:52.222] Applying learner 'classif.kknn' on task 'spirals_task' (iter 47/100)
## INFO  [10:24:52.245] Applying learner 'classif.kknn' on task 'spirals_task' (iter 48/100)
## INFO  [10:24:52.268] Applying learner 'classif.kknn' on task 'spirals_task' (iter 49/100)
## INFO  [10:24:52.291] Applying learner 'classif.kknn' on task 'spirals_task' (iter 50/100)
## INFO  [10:24:52.313] Applying learner 'classif.kknn' on task 'spirals_task' (iter 51/100)
## INFO  [10:24:52.336] Applying learner 'classif.kknn' on task 'spirals_task' (iter 52/100)
## INFO  [10:24:52.368] Applying learner 'classif.kknn' on task 'spirals_task' (iter 53/100)
## INFO  [10:24:52.397] Applying learner 'classif.kknn' on task 'spirals_task' (iter 54/100)
## INFO  [10:24:52.420] Applying learner 'classif.kknn' on task 'spirals_task' (iter 55/100)
## INFO  [10:24:52.444] Applying learner 'classif.kknn' on task 'spirals_task' (iter 56/100)
## INFO  [10:24:52.467] Applying learner 'classif.kknn' on task 'spirals_task' (iter 57/100)
## INFO  [10:24:52.490] Applying learner 'classif.kknn' on task 'spirals_task' (iter 58/100)
## INFO  [10:24:52.512] Applying learner 'classif.kknn' on task 'spirals_task' (iter 59/100)
## INFO  [10:24:52.535] Applying learner 'classif.kknn' on task 'spirals_task' (iter 60/100)
## INFO  [10:24:52.558] Applying learner 'classif.kknn' on task 'spirals_task' (iter 61/100)
## INFO  [10:24:52.580] Applying learner 'classif.kknn' on task 'spirals_task' (iter 62/100)
## INFO  [10:24:52.603] Applying learner 'classif.kknn' on task 'spirals_task' (iter 63/100)
## INFO  [10:24:52.627] Applying learner 'classif.kknn' on task 'spirals_task' (iter 64/100)
## INFO  [10:24:52.661] Applying learner 'classif.kknn' on task 'spirals_task' (iter 65/100)
## INFO  [10:24:52.689] Applying learner 'classif.kknn' on task 'spirals_task' (iter 66/100)
## INFO  [10:24:52.711] Applying learner 'classif.kknn' on task 'spirals_task' (iter 67/100)
## INFO  [10:24:52.735] Applying learner 'classif.kknn' on task 'spirals_task' (iter 68/100)
## INFO  [10:24:52.759] Applying learner 'classif.kknn' on task 'spirals_task' (iter 69/100)
## INFO  [10:24:52.783] Applying learner 'classif.kknn' on task 'spirals_task' (iter 70/100)
## INFO  [10:24:52.808] Applying learner 'classif.kknn' on task 'spirals_task' (iter 71/100)
## INFO  [10:24:52.833] Applying learner 'classif.kknn' on task 'spirals_task' (iter 72/100)
## INFO  [10:24:52.859] Applying learner 'classif.kknn' on task 'spirals_task' (iter 73/100)
## INFO  [10:24:52.893] Applying learner 'classif.kknn' on task 'spirals_task' (iter 74/100)
## INFO  [10:24:52.922] Applying learner 'classif.kknn' on task 'spirals_task' (iter 75/100)
## INFO  [10:24:52.947] Applying learner 'classif.kknn' on task 'spirals_task' (iter 76/100)
## INFO  [10:24:52.974] Applying learner 'classif.kknn' on task 'spirals_task' (iter 77/100)
## INFO  [10:24:53.000] Applying learner 'classif.kknn' on task 'spirals_task' (iter 78/100)
## INFO  [10:24:53.028] Applying learner 'classif.kknn' on task 'spirals_task' (iter 79/100)
## INFO  [10:24:53.055] Applying learner 'classif.kknn' on task 'spirals_task' (iter 80/100)
## INFO  [10:24:53.082] Applying learner 'classif.kknn' on task 'spirals_task' (iter 81/100)
## INFO  [10:24:53.109] Applying learner 'classif.kknn' on task 'spirals_task' (iter 82/100)
## INFO  [10:24:53.135] Applying learner 'classif.kknn' on task 'spirals_task' (iter 83/100)
## INFO  [10:24:53.161] Applying learner 'classif.kknn' on task 'spirals_task' (iter 84/100)
## INFO  [10:24:53.187] Applying learner 'classif.kknn' on task 'spirals_task' (iter 85/100)
## INFO  [10:24:53.212] Applying learner 'classif.kknn' on task 'spirals_task' (iter 86/100)
## INFO  [10:24:53.235] Applying learner 'classif.kknn' on task 'spirals_task' (iter 87/100)
## INFO  [10:24:53.258] Applying learner 'classif.kknn' on task 'spirals_task' (iter 88/100)
## INFO  [10:24:53.282] Applying learner 'classif.kknn' on task 'spirals_task' (iter 89/100)
## INFO  [10:24:53.304] Applying learner 'classif.kknn' on task 'spirals_task' (iter 90/100)
## INFO  [10:24:53.327] Applying learner 'classif.kknn' on task 'spirals_task' (iter 91/100)
## INFO  [10:24:53.349] Applying learner 'classif.kknn' on task 'spirals_task' (iter 92/100)
## INFO  [10:24:53.373] Applying learner 'classif.kknn' on task 'spirals_task' (iter 93/100)
```

```
## INFO  [10:24:53.395] Applying learner 'classif.kknn' on task 'spirals_task' (iter 94/100)
## INFO  [10:24:53.427] Applying learner 'classif.kknn' on task 'spirals_task' (iter 95/100)
## INFO  [10:24:53.455] Applying learner 'classif.kknn' on task 'spirals_task' (iter 96/100)
## INFO  [10:24:53.478] Applying learner 'classif.kknn' on task 'spirals_task' (iter 97/100)
## INFO  [10:24:53.502] Applying learner 'classif.kknn' on task 'spirals_task' (iter 98/100)
## INFO  [10:24:53.525] Applying learner 'classif.kknn' on task 'spirals_task' (iter 99/100)
## INFO  [10:24:53.548] Applying learner 'classif.kknn' on task 'spirals_task' (iter 100/100)
```

```
mlr_cv$score()[, c("iteration", "classif.ce")]
```

```
##      iteration classif.ce
##   1:         1       0.10
##   2:         2       0.10
##   3:         3       0.02
##   4:         4       0.08
##   5:         5       0.08
##   6:         6       0.06
##   7:         7       0.04
##   8:         8       0.02
##   9:         9       0.10
##  10:        10       0.10
##  11:        11       0.14
##  12:        12       0.04
##  13:        13       0.10
##  14:        14       0.04
##  15:        15       0.08
##  16:        16       0.04
##  17:        17       0.04
##  18:        18       0.08
##  19:        19       0.04
##  20:        20       0.08
##  21:        21       0.10
##  22:        22       0.04
##  23:        23       0.02
##  24:        24       0.10
##  25:        25       0.06
##  26:        26       0.06
##  27:        27       0.02
##  28:        28       0.10
##  29:        29       0.12
##  30:        30       0.10
##  31:        31       0.10
##  32:        32       0.02
##  33:        33       0.08
##  34:        34       0.10
##  35:        35       0.08
##  36:        36       0.06
##  37:        37       0.06
##  38:        38       0.08
##  39:        39       0.06
##  40:        40       0.06
##  41:        41       0.08
##  42:        42       0.04
##  43:        43       0.08
```

```
##  44:        44       0.10
##  45:        45       0.04
##  46:        46       0.04
##  47:        47       0.04
##  48:        48       0.12
##  49:        49       0.08
##  50:        50       0.04
##  51:        51       0.06
##  52:        52       0.08
##  53:        53       0.04
##  54:        54       0.08
##  55:        55       0.08
##  56:        56       0.04
##  57:        57       0.12
##  58:        58       0.00
##  59:        59       0.08
##  60:        60       0.06
##  61:        61       0.08
##  62:        62       0.06
##  63:        63       0.04
##  64:        64       0.08
##  65:        65       0.04
##  66:        66       0.02
##  67:        67       0.06
##  68:        68       0.06
##  69:        69       0.12
##  70:        70       0.08
##  71:        71       0.08
##  72:        72       0.04
##  73:        73       0.02
##  74:        74       0.08
##  75:        75       0.14
##  76:        76       0.06
##  77:        77       0.04
##  78:        78       0.02
##  79:        79       0.14
##  80:        80       0.06
##  81:        81       0.12
##  82:        82       0.02
##  83:        83       0.02
##  84:        84       0.04
##  85:        85       0.08
##  86:        86       0.04
##  87:        87       0.06
##  88:        88       0.14
##  89:        89       0.10
##  90:        90       0.06
##  91:        91       0.12
##  92:        92       0.12
##  93:        93       0.04
##  94:        94       0.08
##  95:        95       0.08
##  96:        96       0.06
##  97:        97       0.02
```

```
##  98:         98       0.06
##  99:         99       0.02
## 100:        100       0.08
##       iteration classif.ce
```

```
mlr_cv$aggregate()
```

```
## classif.ce
##     0.0678
```

```
library(ggplot2)

ggplot(data = mlr_cv$score()[, "classif.ce"], aes(y = classif.ce, x = 1)) +
  geom_boxplot() +
  ggtitle(label = "Repeated CV (10-10) with mlr") +
  xlab("") + ylab("test error") + xlim(c(0, 2))
```