Introduction to mlr

Beginner Workshop

Janek Thomas, Daniel Schalk

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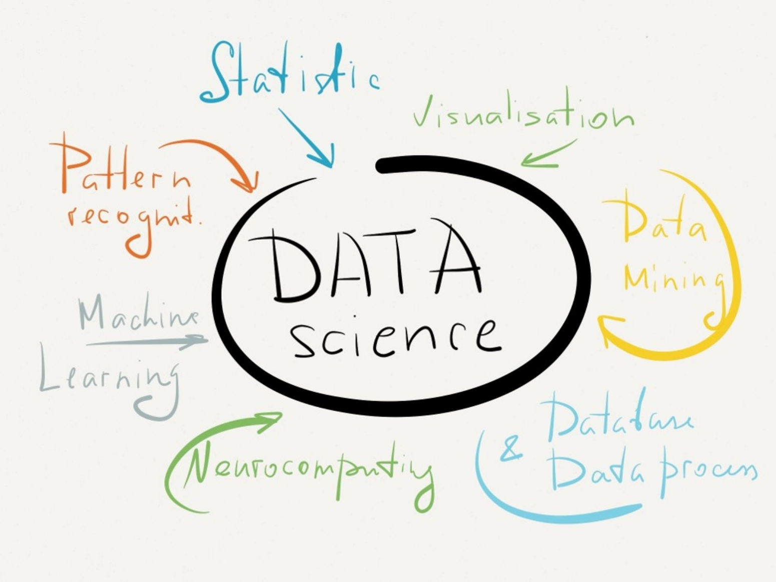
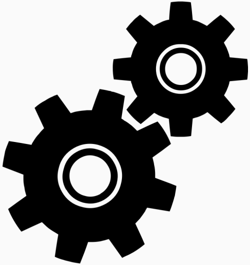
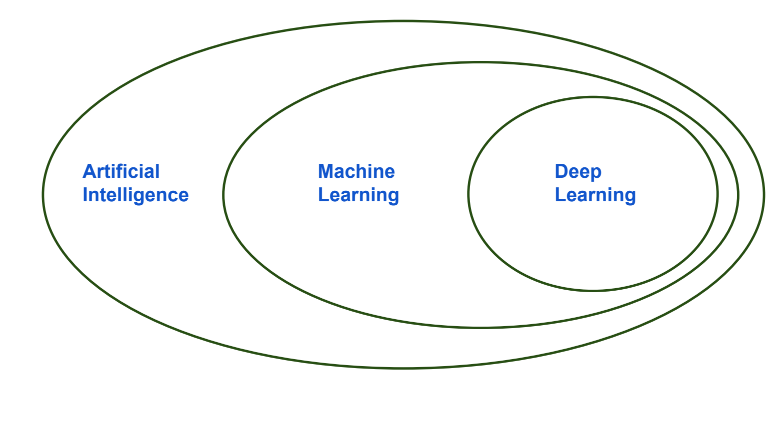
WHAT IS MACHINE LEARNING

DATA SCIENCE AND MACHINE LEARNING





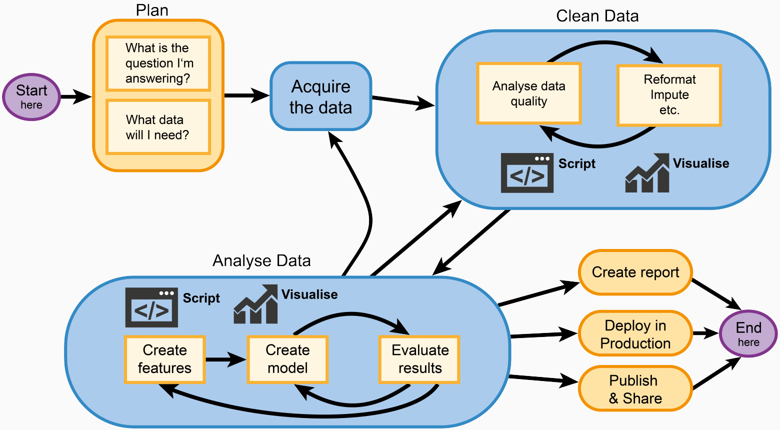
Machine Learning is a method of teaching computers to make predictions based on some data.


Artificial
Intelligence
Machine
Learning
Deep
Learning

MACHINE LEARNING IS CHANGING OUR WORLD

- Search engines learn what you want
- Recommender systems learn your taste in books, music, movies,...
- Algorithms do automatic stock trading
- Elections are won by understanding voters
- Google Translate learns how to translate text
- Siri learns to understand speech
- DeepMind beats humans at Go
- Cars drive themselves
- Medicines are developed faster
- Smartwatches monitor your health
- Data-driven discoveries are made in Physics, Biology, Genetics, Astronomy, Chemistry, Neurology, ...

MOTIVATION


Plan
What is the question I'm answering?
What data will I need?
Start here
Acquire the data
Clean Data
Analyse data quality
Reformat Impute etc.
Script
Visualise
Analyse Data
Script
Visualise
Create features
Create model
Evaluate results
Create report
Deploy in Production
Publish & Share
End here

MLR AND A FIRST EXAMPLE

MOTIVATION: MACHINE LEARNING IN R

The **good** news:

- CRAN serves hundreds of packages for machine learning
- Often compliant to the unwritten interface definition:

```
model = fit(target ~ ., data = train.data, ...)
predictions = predict(model, newdata = test.data, ...)
```

The **bad** news:

- Some packages' API is "just different"
- Functionality is always package or model-dependent, even though the procedure might be general
- No meta-information available or buried in docs

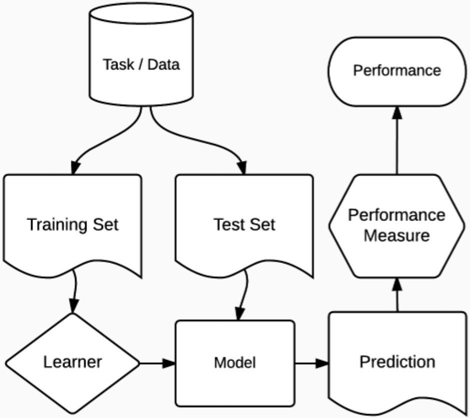
Our goal: A domain-specific language for ML concepts!

MOTIVATION: MLR

- Project home page: https://github.com/mlr-org/mlr
    - Cheatsheet for an quick overview
    - Tutorial for mlr documentation with many code examples
    - Ask questions in the GitHub issue tracker
- 8-10 main developers, quite a few contributors, 4 GSOC projects in 2015/16 and one coming in 2017
- About 30K lines of code, 8K lines of unit tests

MOTIVATION: MLR

- Unified interface for the basic building blocks: tasks, learners, hyperparameters, ...



FEATURES OF MLR

- **Tasks and Learners**
- **Train, Test, Resample**
- **Performance**
- **Benchmarking**
- Hyperparameter Tuning
- Nested Resampling
- Parallelization

LEARN MORE

- Extensive Tutorial covers *all* features in mlr:
  https://mlr-org.github.io/mlr/
- Tuning
- Resampling (with blocking)
- Visualization Topics
- Multilabel Classification, Survival Analysis, Clustering
- Handling Spatial Data
- Functional Data
- Create Custom Learners and Measures
- ...

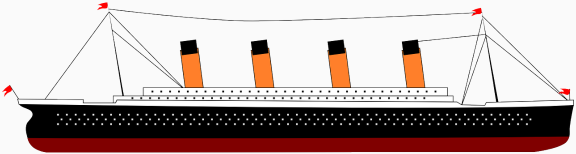
GETTING HELP

- Ask questions on Stackoverflow: https://stackoverflow.com/questions/tagged/mlr
- Found bugs? Report them: https://github.com/mlr-org/mlr/issues

You want to contribute? - Open a PR on github and join our slack: https://mlr-org.slack.com/

TITANIC - MACHINE LEARNING FROM DISASTER

- Titanic sinking on April 15, 1912
- Data provided on Kaggle:
  https://www.kaggle.com/c/titanic
- 809 out of 1309 passengers died
- Task:
  - Can we predict who survived?
  - Why did people die / Which groups?



TITANIC - DATA SET

Data Dictionary:

`Survived`	Survived, 0 = No, 1 = Yes
`Pclass`	Ticket class, from 1st to 3rd
`Sex`	Sex
`Age`	Age in years
`Sibsp`	# of siblings/ spouses
`Parch`	# of parents/ children
`Ticket`	Ticket number
`Fare`	Passenger fare
`Cabin`	Cabin number
`Embarked`	Port of Embarkation

TITANIC - DATA SET

```
load("titanic.rda")
str(data)

## 'data.frame':    1309 obs. of  11 variables:
##  $ Pclass  : Factor w/ 3 levels "1","2","3": 1 1 1 1 1 1 1 1 ...
##  $ Survived: Factor w/ 2 levels "0","1": 2 2 1 1 1 2 2 1 ...
##  $ Name    : chr  "Allen, Miss. Elisabeth Walton" "Allison, Ma"..
##  $ Sex     : Factor w/ 2 levels "female","male": 1 2 1 2 1 2 1 ..
##  $ Age     : num  29 0.917 2 30 ...
##  $ Sibsp   : num  0 1 1 1 1 0 1 0 ...
##  $ Parch   : num  0 2 2 2 2 0 0 0 ...
##  $ Ticket  : Factor w/ 929 levels "110152","110413",..: 188 50 ..
##  $ Fare    : num  211 152 152 152 ...
##  $ Cabin   : Factor w/ 187 levels "","A10","A11",..: 45 81 81 8..
##  $ Embarked: Factor w/ 4 levels "","C","Q","S": 4 4 4 4 4 4 4 4..
```

TITANIC - DATA SET

```
library(mlr)
print(summarizeColumns(data)[, -c(5, 6, 7)], digits = 0)

##        name      type  na mean min  max nlevs
## 1    Pclass    factor   0   NA 277  709     3
## 2  Survived    factor   0   NA 500  809     2
## 3      Name character   0   NA   1    2  1307
## 4       Sex    factor   0   NA 466  843     2
## 5       Age   numeric 263   30   0   80     0
## 6     Sibsp   numeric   0    0   0    8     0
## 7     Parch   numeric   0    0   0    9     0
## 8    Ticket    factor   0   NA   1   11   929
## 9      Fare   numeric   1   33   0  512     0
## 10    Cabin    factor   0   NA   1 1014   187
## 11 Embarked    factor   0   NA   2  914     4
```

TITANIC - PREPROCESSING

Set empty factor levels to NA:

```
data$Embarked[data$Embarked == ""] = NA
data$Embarked = droplevels(data$Embarked)
data$Cabin[data$Cabin == ""] = NA
data$Cabin = droplevels(data$Cabin)
```

TITANIC - PREPROCESSING

```r
library(BBmisc)
library(stringi)

# Price per person, multiple tickets bought by one person
data$farePp = data$Fare / (data$Parch + data$Sibsp + 1)

# The deck can be extracted from the the cabin number
data$deck = as.factor(stri_sub(data$Cabin, 1, 1))

# Starboard had an odd number, portside even cabin numbers
data$portside = stri_extract_last_regex(data$Cabin, "[0-9]")
data$portside = as.numeric(data$portside) %% 2

# Drop stuff we cannot easily model on
data = dropNamed(data,
  c("Cabin","PassengerId", "Ticket", "Name"))
```

TITANIC - PREPROCESSING

```
print(summarizeColumns(data)[, -c(5, 6, 7)], digits = 0)

##         name    type   na mean min max nlevs
## 1     Pclass  factor    0   NA 277 709     3
## 2   Survived  factor    0   NA 500 809     2
## 3        Sex  factor    0   NA 466 843     2
## 4        Age numeric  263   30   0  80     0
## 5      Sibsp numeric    0    0   0   8     0
## 6      Parch numeric    0    0   0   9     0
## 7       Fare numeric    1   33   0 512     0
## 8   Embarked  factor    2   NA 123 914     3
## 9     farePp numeric    1   21   0 512     0
## 10      deck  factor 1014   NA   1  94     8
## 11 portside numeric 1020    0   0   1     0
```

TITANIC - PREPROCESSING

- Impute missing numeric values with median, missing factor values with a separate category
- NB: This is really naive, we should probably embed this in cross-validation

```
data = impute(data, cols = list(
  Age = imputeMedian(),
  Fare = imputeMedian(),
  Embarked = imputeConstant("__miss__"),
  farePp = imputeMedian(),
  deck = imputeConstant("__miss__"),
  portside = imputeConstant("__miss__")
))

data = data$data
data = convertDataFrameCols(data, chars.as.factor = TRUE)
```

TITANIC - TASK

```
task = makeClassifTask(id = "titanic", data = data,
  target = "Survived", positive = "1")
print(task)

## Supervised task: titanic
## Type: classif
## Target: Survived
## Observations: 1309
## Features:
##    numerics     factors     ordered functionals
##           5           5           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
## Classes: 2
##   0   1
## 809 500
## Positive class: 1
```

WHAT LEARNERS ARE AVAILABLE?

Classification

- LDA, QDA, RDA, MDA
- Trees and forests
- Boosting (different variants)
- SVMs (different variants)
- (Deep) Neural Networks
- ...

Regression

- Linear, lasso and ridge
- Boosting
- Trees and forests
- Gaussian processes
- (Deep) Neural Networks
- ...

Clustering

- K-Means
- EM
- DBscan
- X-Means
- ...

Survival

- Cox-PH
- Cox-Boost
- Random survival forest
- Penalized regression
- ...

WHAT LEARNERS ARE AVAILABLE?

We can explore them on the webpage:

mlr 2.13 Get Started Basics Advanced Extending Appendix mlr-org Packages Search...

Class / Short Name / Name	Packages	Num.	Fac.	Ord.	NAs	Weights	Props	Note
classif.ada *ada* ada Boosting	ada rpart	X	X				prob twoclass	`xval` has been set to `0` by default for spee
classif.adaboostm1 *adaboostm1* ada Boosting M1	RWeka	X	X				prob twoclass multiclass	NAs are directly passed to WEKA with `na.ac`
classif.bartMachine *bartmachine* Bayesian Additive Regression Trees	bartMachine	X	X		X		prob twoclass	`use_missing_data` has been set to `TRUE`
classif.binomial *binomial* Binomial Regression	stats	X	X			X	prob twoclass	Delegates to `glm` with freely choosable bin

WHAT LEARNERS ARE AVAILABLE?

Or ask mlr

```
tab = listLearners(task, warn.missing.packages = FALSE)
tab[1:5, c("class", "package")]

##                   class      package
## 1 classif.adaboostm1        RWeka
## 2   classif.binomial        stats
## 3 classif.blackboost mboost,party
## 4    classif.cforest        party
## 5      classif.ctree        party
```

TITANIC - LEARNER

```
lrn = makeLearner("classif.kknn", k = 3, predict.type = "prob")
print(lrn)

## Learner classif.kknn from package kknn
## Type: classif
## Name: k-Nearest Neighbor; Short name: kknn
## Class: classif.kknn
## Properties: twoclass,multiclass,numerics,factors,prob
## Predict-Type: prob
## Hyperparameters: k=3
```

TITANIC - TRAIN

```
set.seed(123)
n = getTaskSize(task)
train = sample(n, size = 2/3 * n)
test = setdiff(1:n, train)

head(sort(train))

## [1] 1 2 3 5 7 9

head(sort(test))

## [1]  4  6  8 11 12 18

mod = train(lrn, task, subset = train)
```

TITANIC - MODEL

```
print(mod)

## Model for learner.id=classif.kknn; learner.class=classif.kknn
## Trained on: task.id = titanic; obs = 872; features = 10
## Hyperparameters: k=3

# retrieve model as returned from the third party package
# [NB: knn does not have a training step, mlr just returns the
#  training data which is required in the predict step]
rmodel = getLearnerModel(mod)
```

TITANIC - PREDICT

```
pred = predict(mod, task = task, subset = test)
head(as.data.frame(pred))

##    id truth prob.0 prob.1 response
## 4   4     0 0.6621  0.338        0
## 6   6     1 0.7358  0.264        0
## 8   8     0 1.0000  0.000        0
## 11 11     0 0.7358  0.264        0
## 12 12     1 0.0000  1.000        1
## 18 18     1 0.0737  0.926        1

head(getPredictionProbabilities(pred))

## [1] 0.338 0.264 0.000 0.264 1.000 0.926
```

TITANIC - PERFORMANCE

```
performance(pred, measures = list(mlr::acc, mlr::auc))

##   acc   auc
## 0.725 0.786
```

TITANIC - EXTERNAL VALIDATION SET

You can also predict on data not included in the task:

```
test.data = dropNamed(data[test, ], "Survived")
pred = predict(mod, newdata = data[test, ])
performance(pred, measures = list(mlr::acc, mlr::auc))

##   acc   auc
## 0.725 0.786
```

NOTEBOOK 1

RESAMPLING

PARAMETER OF MAKERESAMPLINGDESC

Methods	Parameter
`CV`	`iters` (Number of iterations)
`LOO`	
`RepCV`	`reps` (Repeats for repeated CV)
	`folds` (Folds in the repeated CV)
`Bootstrap`	`iters` (Number of iterations)
`Subsample`	`iters` (Number of iterations)
	`split` (Proportion of training cases)
`Holdout`	`split` (Proportion of training cases)

For instance 10-fold cross validation:

```
makeResampleDesc(method = "CV", iters = 10)

## Resample description: cross-validation with 10 iterations.
## Predict: test
## Stratification: FALSE
```

POSSIBLE WAYS TO USE CROSS VALIDATION

1. Explicitly define resampling:

```
rdesc = makeResampleDesc("CV", iters = 10)
rdesc = cv10

res1 = resample("classif.randomForest", iris.task, resampling = rdesc,
  show.info = FALSE)
res2 = resample("classif.randomForest", iris.task, resampling = cv10,
  show.info = FALSE)

res1
```

```
## Resample Result
## Task: iris-example
## Learner: classif.randomForest
## Aggr perf: mmce.test.mean=0.047
## Runtime: 0.42655
```

Other pre defined objects are `cv2`, `cv3` and `cv5`.

POSSIBLE WAYS TO USE CROSS VALIDATION

2. Use `crossval`:

```r
res3 = crossval("classif.randomForest", iris.task, iters = 10,
  show.info = FALSE)
res3
```

```
## Resample Result
## Task: iris-example
## Learner: classif.randomForest
## Aggr perf: mmce.test.mean=0.053
## Runtime: 0.358441
```

Similar functions are `repcv`, `holdoud`, `subsample`, `bootstrapOOB`, `bootstrapB632` and `bootstrapB632plus`.

CLASSIFICATION ANALYSIS: BENCHMARKING

```r
# quick way to compare learners with identical train/test splits
task = iris.task
learners = list(
  makeLearner("classif.knn", k = 3),
  makeLearner("classif.lda"),
  makeLearner("classif.naiveBayes")
)
benchmark(learners, task, resamplings = cv3)

##        task.id         learner.id mmce.test.mean
## 1 iris-example        classif.knn           0.04
## 2 iris-example        classif.lda           0.02
## 3 iris-example classif.naiveBayes           0.04
```

CLASSIFICATION ANALYSIS: BENCHMARKING

```
tasks = list(iris.task, sonar.task, pid.task)
bm = benchmark(learners, tasks, resampling = cv3)
print(bm)

##                      task.id         learner.id mmce.test.mean
## 1               iris-example        classif.knn         0.0333
## 2               iris-example        classif.lda         0.0200
## 3               iris-example classif.naiveBayes         0.0400
## 4 PimaIndiansDiabetes-example        classif.knn         0.3021
## 5 PimaIndiansDiabetes-example        classif.lda         0.2253
## 6 PimaIndiansDiabetes-example classif.naiveBayes         0.2448
## 7              Sonar-example        classif.knn         0.2207
## 8              Sonar-example        classif.lda         0.2355
## 9              Sonar-example classif.naiveBayes         0.3226
```

CLASSIFICATION ANALYSIS: BENCHMARKING

```r
# aggregated data:
getBMRAggrPerformances(bm, as.df = TRUE)

##                        task.id         learner.id mmce.test.mean
## 1                 iris-example       classif.knn         0.0333
## 2                 iris-example       classif.lda         0.0200
## 3                 iris-example classif.naiveBayes         0.0400
## 4 PimaIndiansDiabetes-example       classif.knn         0.3021
## 5 PimaIndiansDiabetes-example       classif.lda         0.2253
## 6 PimaIndiansDiabetes-example classif.naiveBayes         0.2448
## 7                Sonar-example       classif.knn         0.2207
## 8                Sonar-example       classif.lda         0.2355
## 9                Sonar-example classif.naiveBayes         0.3226
```

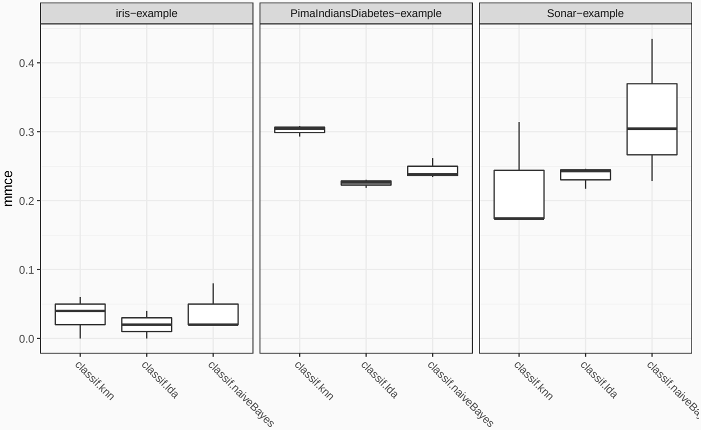
CLASSIFICATION ANALYSIS: BENCHMARKING

```r
# complete data:
head(as.data.frame(bm), 10)

##                           task.id         learner.id iter  mmce
## 1                    iris-example        classif.knn    1 0.040
## 2                    iris-example        classif.knn    2 0.060
## 3                    iris-example        classif.knn    3 0.000
## 4                    iris-example        classif.lda    1 0.020
## 5                    iris-example        classif.lda    2 0.040
## 6                    iris-example        classif.lda    3 0.000
## 7                    iris-example classif.naiveBayes    1 0.020
## 8                    iris-example classif.naiveBayes    2 0.080
## 9                    iris-example classif.naiveBayes    3 0.020
## 10 PimaIndiansDiabetes-example        classif.knn    1 0.309
```

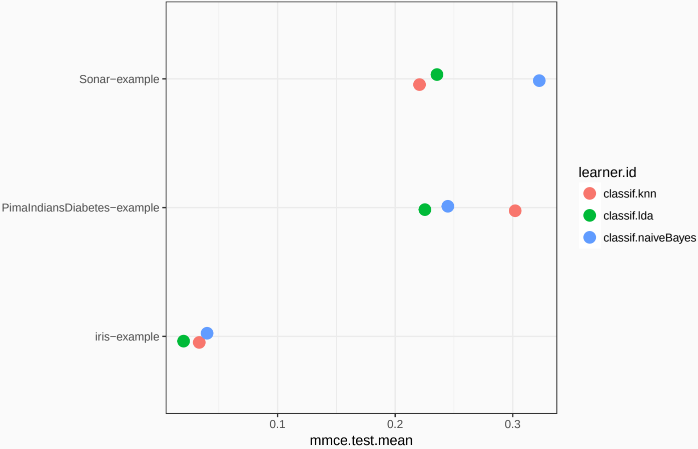
CLASSIFICATION ANALYSIS: BENCHMARKING

```
plotBMRBoxplots(bm, pretty.names = FALSE)
```



CLASSIFICATION ANALYSIS: BENCHMARKING

```r
plotBMRSummary(bm, pretty.names = FALSE)
```



TUNING

```
lrn = makeLearner("classif.rpart")
getParamSet(lrn)

##                    Type len  Def   Constr Req Tunable Trafo
## minsplit        integer   -   20 1 to Inf   -    TRUE     -
## minbucket       integer   -    - 1 to Inf   -    TRUE     -
## cp              numeric   - 0.01   0 to 1   -    TRUE     -
## maxcompete      integer   -    4 0 to Inf   -    TRUE     -
## maxsurrogate    integer   -    5 0 to Inf   -    TRUE     -
## usesurrogate   discrete   -    2    0,1,2   -    TRUE     -
## surrogatestyle discrete   -    0      0,1   -    TRUE     -
## maxdepth        integer   -   30  1 to 30   -    TRUE     -
## xval            integer   -   10 0 to Inf   -   FALSE     -
## parms           untyped   -    -        -   -    TRUE     -
```

HYPERPARAMETERS IN MLR

Either set them in constructor, or change them later:

```
lrn = makeLearner("classif.ksvm", C = 5, sigma = 3)
lrn = setHyperPars(lrn, C = 1, sigma = 2)
lrn$par.vals

## $fit
## [1] FALSE
##
## $C
## [1] 1
##
## $sigma
## [1] 2
```

TUNING IN MLR

- Create a set of parameters
- Here we optimize a SVM with radial kernel on logscale

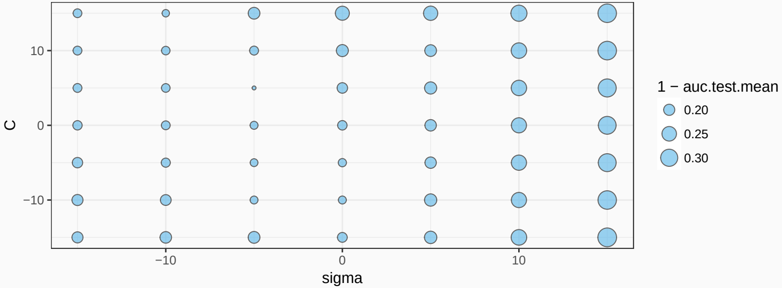
```
lrn = makeLearner("classif.ksvm",
  predict.type = "prob")

par.set = makeParamSet(
  makeNumericParam("C", lower = -8, upper = 8,
    trafo = function(x) 2^x),
  makeNumericParam("sigma", lower = -8, upper = 8,
    trafo = function(x) 2^x)
)
```

GRID SEARCH

Try all combinations of finite grid

$\rightsquigarrow$ Inefficient, combinatorial explosion, searches irrelevant areas

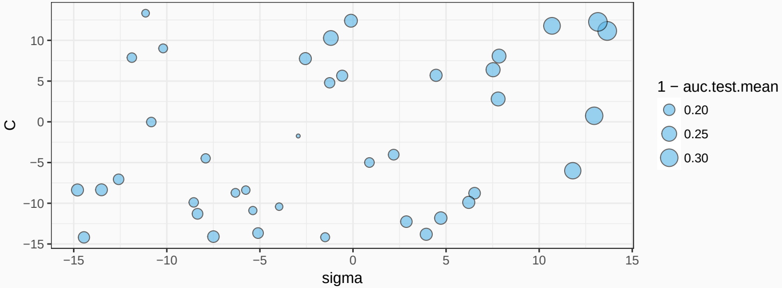



```
ctrl.grid = makeTuneControlGrid(resolution = 7L)
```

RANDOM SEARCH

Uniformly randomly draw configurations

⇝ Scales better then grid search, easily extensible




```r
tune.ctrl = makeTuneControlRandom(maxit = 50L)
```

DEFINING A TEST SET

As for resampling we also need to define how a model is evaluated:

```
res.desc = makeResampleDesc(method = "Holdout")
res.desc

## Resample description: holdout with 0.67 split rate.
## Predict: test
## Stratification: FALSE
```

Optimize the hyperparameter of learner

```
tune.ctrl = makeTuneControlRandom(maxit = 50L)
res = tuneParams(lrn, task = iris.task, par.set = par.set,
  resampling = res.desc, control = tune.ctrl)
```

TUNING IN MLR

- Get best results:

```
res$x

## $C
## [1] 226
##
## $sigma
## [1] 0.00761

res$y

## mmce.test.mean
##           0.04
```

- Get data frame of all 50 iterations:

```
head(as.data.frame(res$opt.path))[, c(1,2,3,7)]

##        C  sigma mmce.test.mean exec.time
## 1   7.82  -7.04           0.04     0.054
## 2 -12.05 -11.04           0.72     0.059
## 3  -2.26   4.83           0.22     0.051
## 4  -6.53   5.51           0.38     0.061
## 5  10.48  -3.42           0.06     0.044
## 6  -3.21   3.51           0.18     0.047
```

NOTEBOOK 2