Full stack data science in R

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Why R? Foundation

1 Full stack data science

2 Data acquisition and processing

3 Model development

4 Model deployment

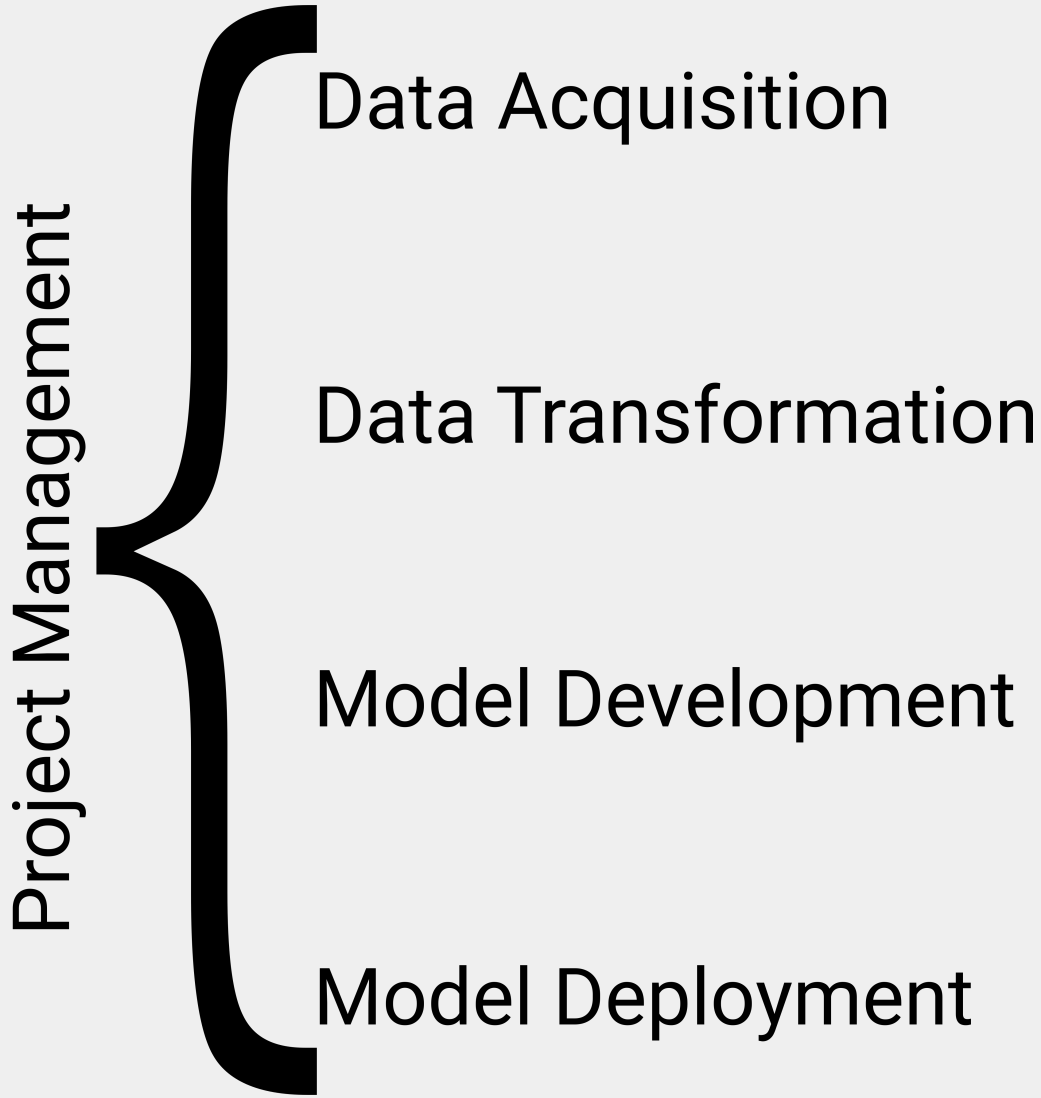
5 Project management

About me

- bioinformatician (Warsaw University of Technology, Brandenburg University of Technology Cottbus-Senftenberg, .prot),
- founder of the Why R? Foundation and Wrocław R User Group,
- facilitator of McKinsey Tech Meetup.

Full stack data science

Full stack data science



Full stack data science in R

Project Management

Data Acquisition

Data Transformation

Model Development

Model Deployment

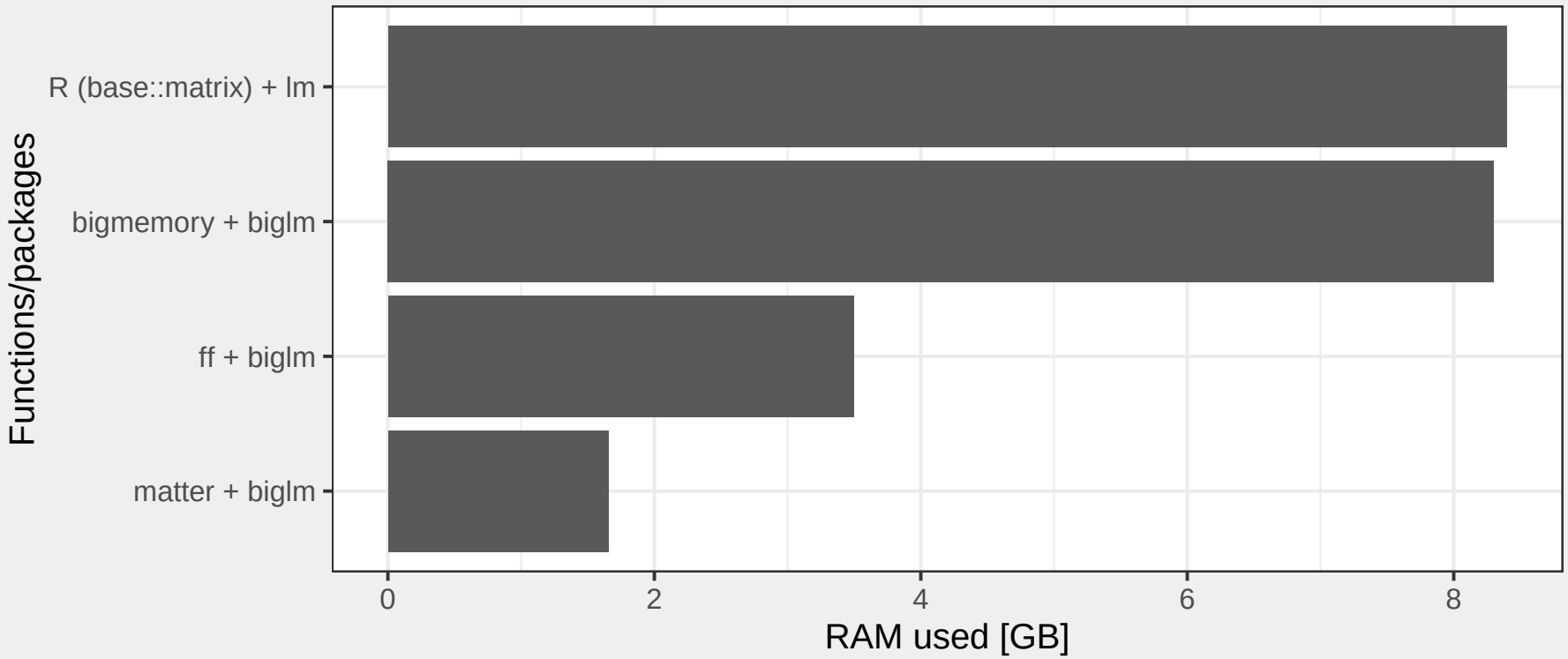
Data acquisition and processing

Data acquisition

Import data to **R** in a *data.frame* (or similar) format.

Type	Package
Tabular	**readr**, **xlsx**, **data.table**::*fread*
Relational databases	**RPostgreSQL**, **mongolite**
Graph databases (e.g., neo4j)	None

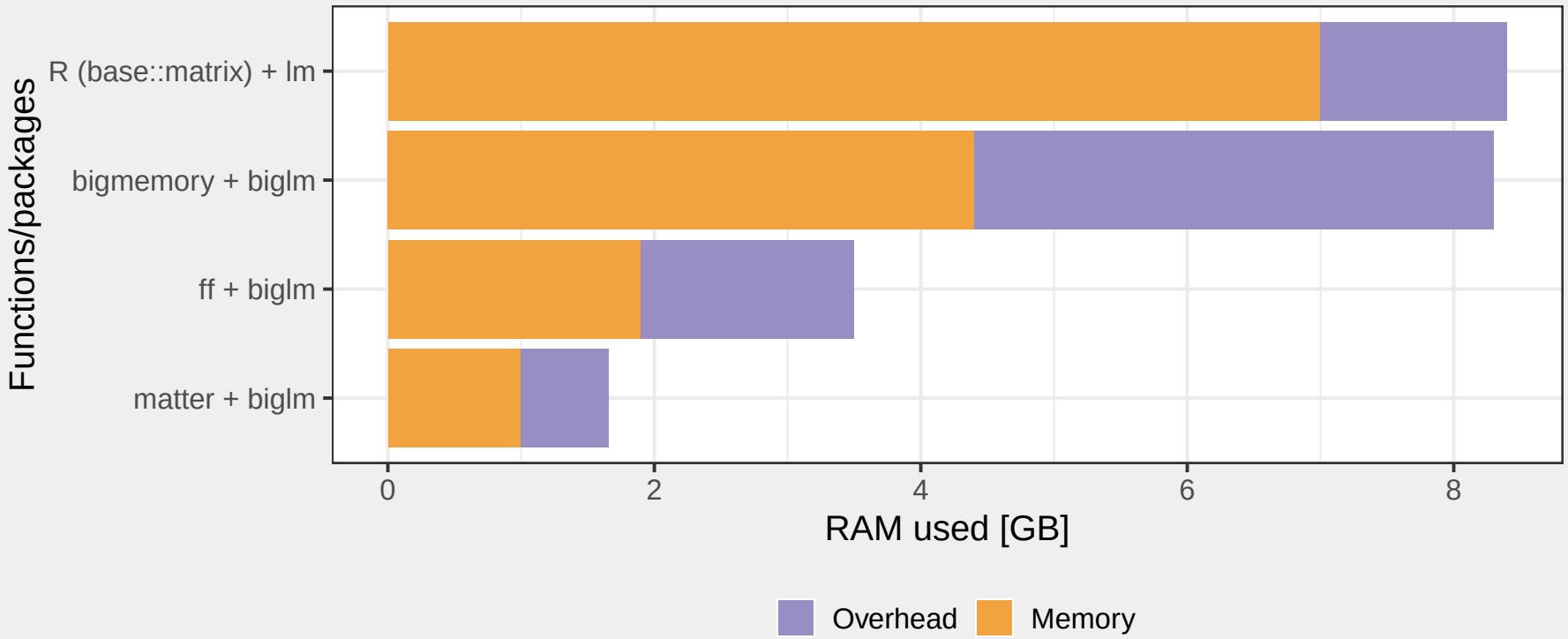
Big data processing



Comparative performance of matter for linear regression and calculation of the first two principal components on simulated datasets of 1.2 GB.

Source: Bemis KA (2019). matter: A framework for rapid prototyping with binary data on disk. R package version 1.10.0, https://github.com/kuwisdelu/matter.

Big data processing



Memory overhead is the maximum memory used during the execution minus the memory in use upon completion.

Source: Bemis KA (2019). matter: A framework for rapid prototyping with binary data on disk. R package version 1.10.0, https://github.com/kuwisdelu/matter.

Model development

MLR

mlr: a standardized interface to machine learning in **R** (by Bernd Bischl and Michael Lang).

Alternatives: **caret**, **parsnip**.

Why mlr?

- amazing documentation,
- separation of learner and task,
- a wide array of tasks: *Classification*, *Regression*, *Cost-sensitive*, Survival, Clustering, Multilabel, Imbalanced data, Functional data, Spatial data.
- 71 performance measures.
- MBO.

MLR TASKS

```
iris[1L:2, ]
```

```
##   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
## 1          5.1         3.5          1.4         0.2  setosa
## 2          4.9         3.0          1.4         0.2  setosa
```

```
iris.task
```

```
## Supervised task: iris-example
## Type: classif
## Target: Species
## Observations: 150
## Features:
##    numerics     factors     ordered functionals
##           4           0           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
## Classes: 3
##     setosa versicolor  virginica
##         50         50         50
## Positive class: NA
```

MLR LEARNERS

```
listLearners()
```

```
##                 class                                    name  short.name
## 1         classif.ada                           ada Boosting         ada
## 2  classif.adaboostm1                      ada Boosting M1  adaboostm1
## 3 classif.bartMachine Bayesian Additive Regression Trees bartmachine
## 4    classif.binomial                  Binomial Regression    binomial
## 5    classif.boosting                      Adabag Boosting      adabag
## 6         classif.bst                    Gradient Boosting         bst
##        package    type installed numerics factors ordered missings weights
## 1    ada,rpart classif     FALSE     TRUE    TRUE   FALSE    FALSE   FALSE
## 2        RWeka classif     FALSE     TRUE    TRUE   FALSE    FALSE   FALSE
## 3  bartMachine classif     FALSE     TRUE    TRUE   FALSE     TRUE   FALSE
## 4        stats classif      TRUE     TRUE    TRUE   FALSE    FALSE    TRUE
## 5 adabag,rpart classif     FALSE     TRUE    TRUE   FALSE     TRUE   FALSE
## 6    bst,rpart classif     FALSE     TRUE   FALSE   FALSE    FALSE   FALSE
##    prob oneclass twoclass multiclass class.weights featimp oobpreds
## 1  TRUE    FALSE     TRUE      FALSE         FALSE   FALSE    FALSE
## 2  TRUE    FALSE     TRUE       TRUE         FALSE   FALSE    FALSE
## 3  TRUE    FALSE     TRUE      FALSE         FALSE   FALSE    FALSE
## 4  TRUE    FALSE     TRUE      FALSE         FALSE   FALSE    FALSE
## 5  TRUE    FALSE     TRUE       TRUE         FALSE    TRUE    FALSE
## 6 FALSE    FALSE     TRUE      FALSE         FALSE   FALSE    FALSE
##   functionals single.functional    se lcens rcens icens
## 1       FALSE             FALSE FALSE FALSE FALSE FALSE
## 2       FALSE             FALSE FALSE FALSE FALSE FALSE
## 3       FALSE             FALSE FALSE FALSE FALSE FALSE
## 4       FALSE             FALSE FALSE FALSE FALSE FALSE
## 5       FALSE             FALSE FALSE FALSE FALSE FALSE
## 6       FALSE             FALSE FALSE FALSE FALSE FALSE
## ... (#rows: 165, #cols: 24)
```

MLR LEARNERS

```
listLearners(obj = iris.task)
```

```
##                 class                                                name
## 1     classif.cforest Random forest based on conditional inference trees
## 2       classif.ctree                          Conditional Inference Trees
## 3 classif.featureless                               Featureless classifier
## 4         classif.fnn                          Fast k-Nearest Neighbour
## 5     classif.gausspr                                Gaussian Processes
## 6         classif.knn                                k-Nearest Neighbor
##    short.name package    type installed numerics factors ordered missings
## 1     cforest   party classif      TRUE     TRUE    TRUE    TRUE     TRUE
## 2       ctree   party classif      TRUE     TRUE    TRUE    TRUE     TRUE
## 3 featureless     mlr classif      TRUE     TRUE    TRUE    TRUE     TRUE
## 4         fnn     FNN classif      TRUE     TRUE   FALSE   FALSE    FALSE
## 5     gausspr kernlab classif      TRUE     TRUE    TRUE   FALSE    FALSE
## 6         knn   class classif      TRUE     TRUE   FALSE   FALSE    FALSE
##   weights  prob oneclass twoclass multiclass class.weights featimp
## 1    TRUE  TRUE    FALSE     TRUE       TRUE         FALSE    TRUE
## 2    TRUE  TRUE    FALSE     TRUE       TRUE         FALSE   FALSE
## 3   FALSE  TRUE    FALSE     TRUE       TRUE         FALSE   FALSE
## 4   FALSE FALSE    FALSE     TRUE       TRUE         FALSE   FALSE
## 5   FALSE  TRUE    FALSE     TRUE       TRUE         FALSE   FALSE
## 6   FALSE FALSE    FALSE     TRUE       TRUE         FALSE   FALSE
##   oobpreds functionals single.functional    se lcens rcens icens
## 1    FALSE       FALSE             FALSE FALSE FALSE FALSE FALSE
## 2    FALSE       FALSE             FALSE FALSE FALSE FALSE FALSE
## 3    FALSE        TRUE             FALSE FALSE FALSE FALSE FALSE
## 4    FALSE       FALSE             FALSE FALSE FALSE FALSE FALSE
## 5    FALSE       FALSE             FALSE FALSE FALSE FALSE FALSE
## 6    FALSE       FALSE             FALSE FALSE FALSE FALSE FALSE
## ... (#rows: 19, #cols: 24)
```

MLR LEARNERS

```r
iris.task <- makeClassifTask(data = iris, target = "Species")

lrn_rng <- makeLearner("classif.ranger")
# ranger: the fastest random forest implementation in R
# Marvin Wright, the author of ranger, is a keynote speaker of Why R? 2019

cv <- makeResampleDesc("CV", iters = 3)

resample(learner = lrn_rng, task = iris.task, resampling = cv)
```

```
## Resampling: cross-validation

## Measures:             mmce

## [Resample] iter 1:    0.0600000

## [Resample] iter 2:    0.0600000

## [Resample] iter 3:    0.0600000

##

## Aggregated Result: mmce.test.mean=0.0600000

##

## Resample Result
## Task: iris
## Learner: classif.ranger
```

Bayesian optimization

$$\max_{x \in \mathbb{R}} f(x)$$

The *posterior* probability of a model (or theory, or hypothesis) M given evidence (or data, or observations) E is proportional to the likelihood of E given M multiplied by the *prior* probability of M:

$$P(M|E) \propto P(E|M)|P(M)$$

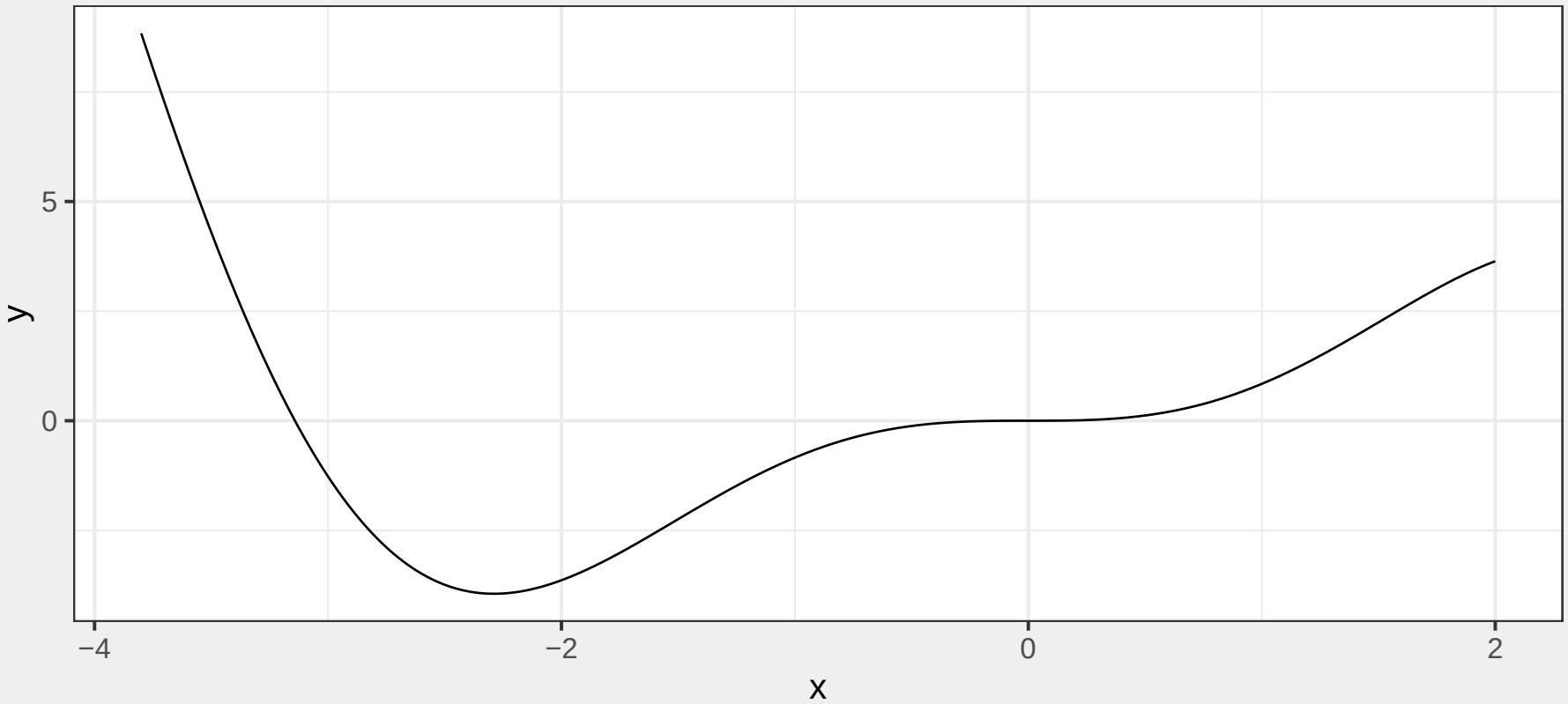
Bayesian optimization

Find local extrema of arbitrary functions.

Bayesian optimization

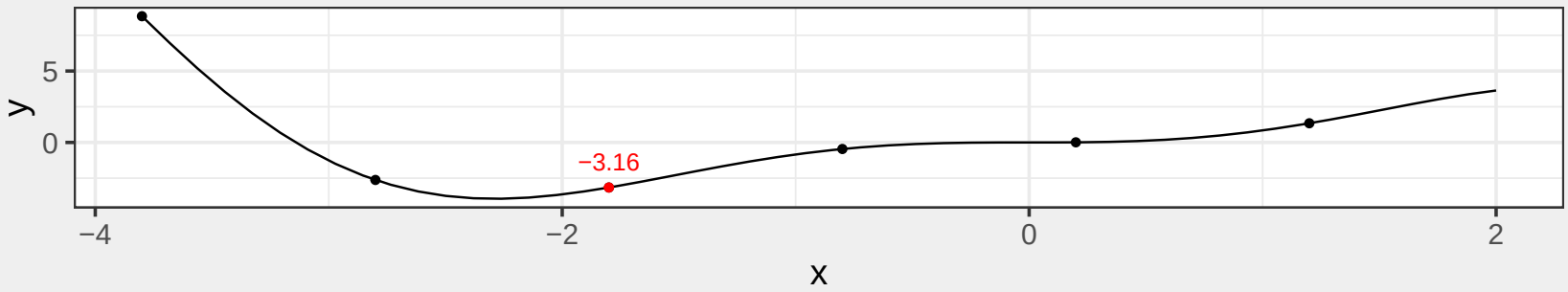
$y = \sin(x) \times x^2$

Local minimum: -3.9453.

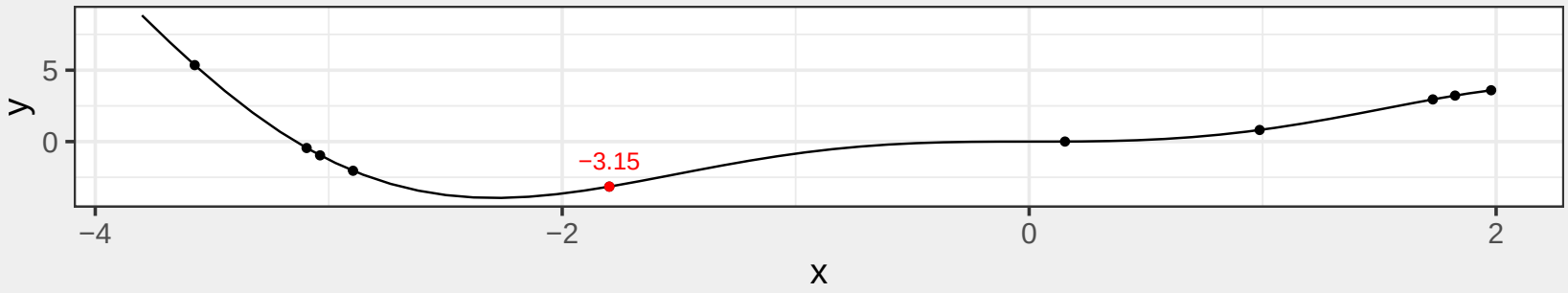


Bayesian optimization

Grid search

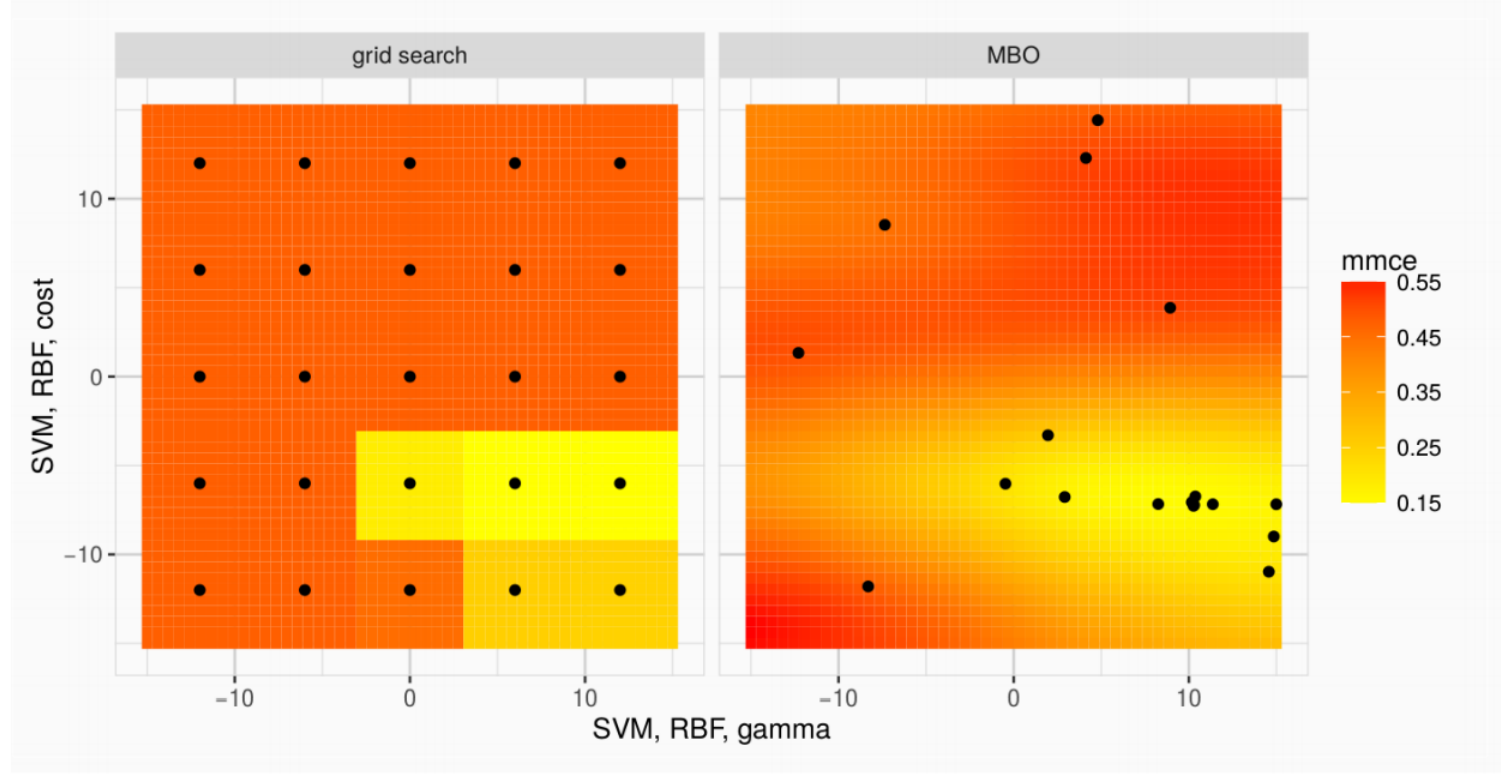


Random search



MBO

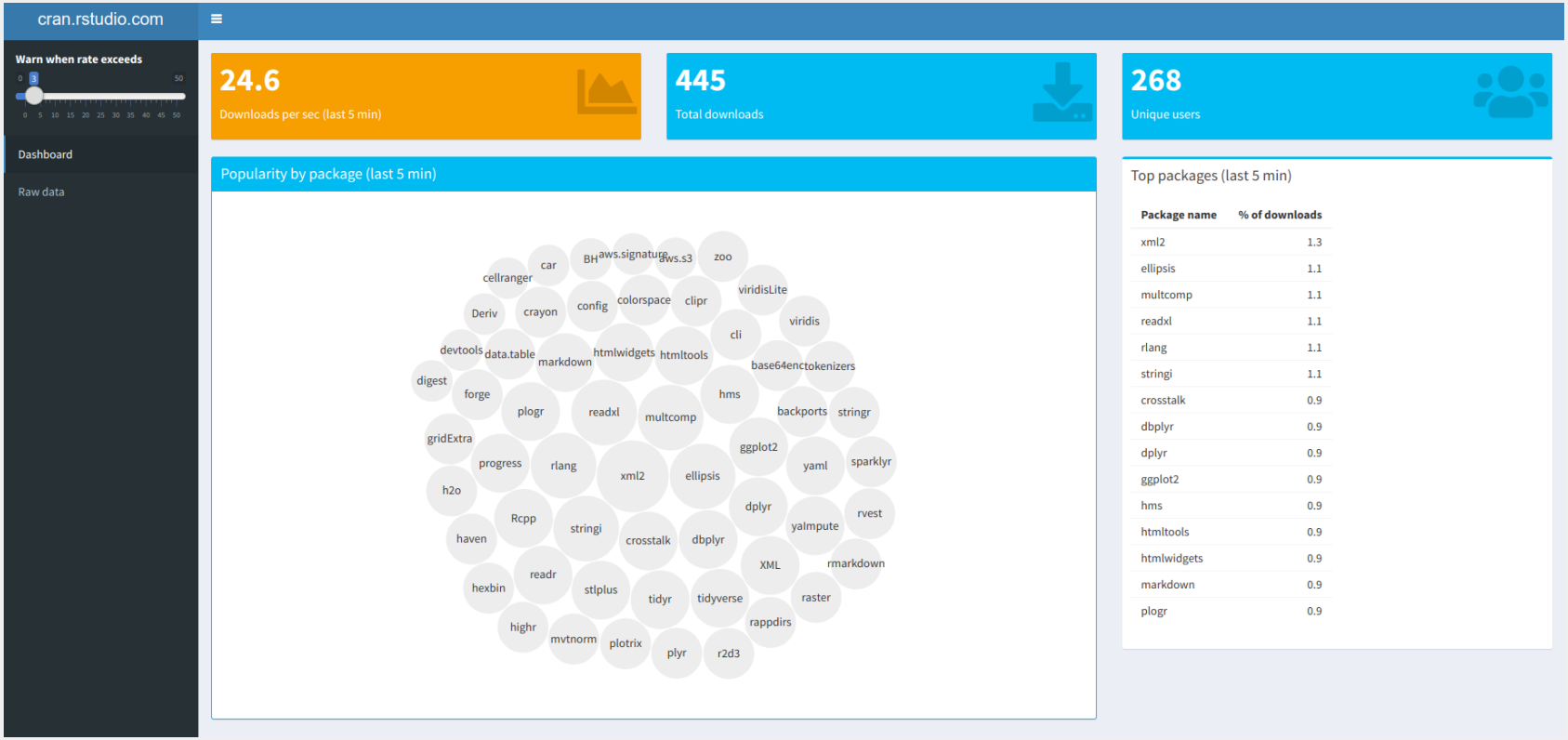
Baysian optimization



Source: Bernd Bischl

Model deployment

Shiny



Limitations:

1. stability decreases with the number of concurrent users,
2. speed.

ShinyProxy and Kubernetes

ShinyProxy: docker-based containers for Shiny apps.

ShinyProxy containers can be themselves run in a container and deployed clustered container managers (such as Kubernetes or Swarm).

Project management

DRAKE

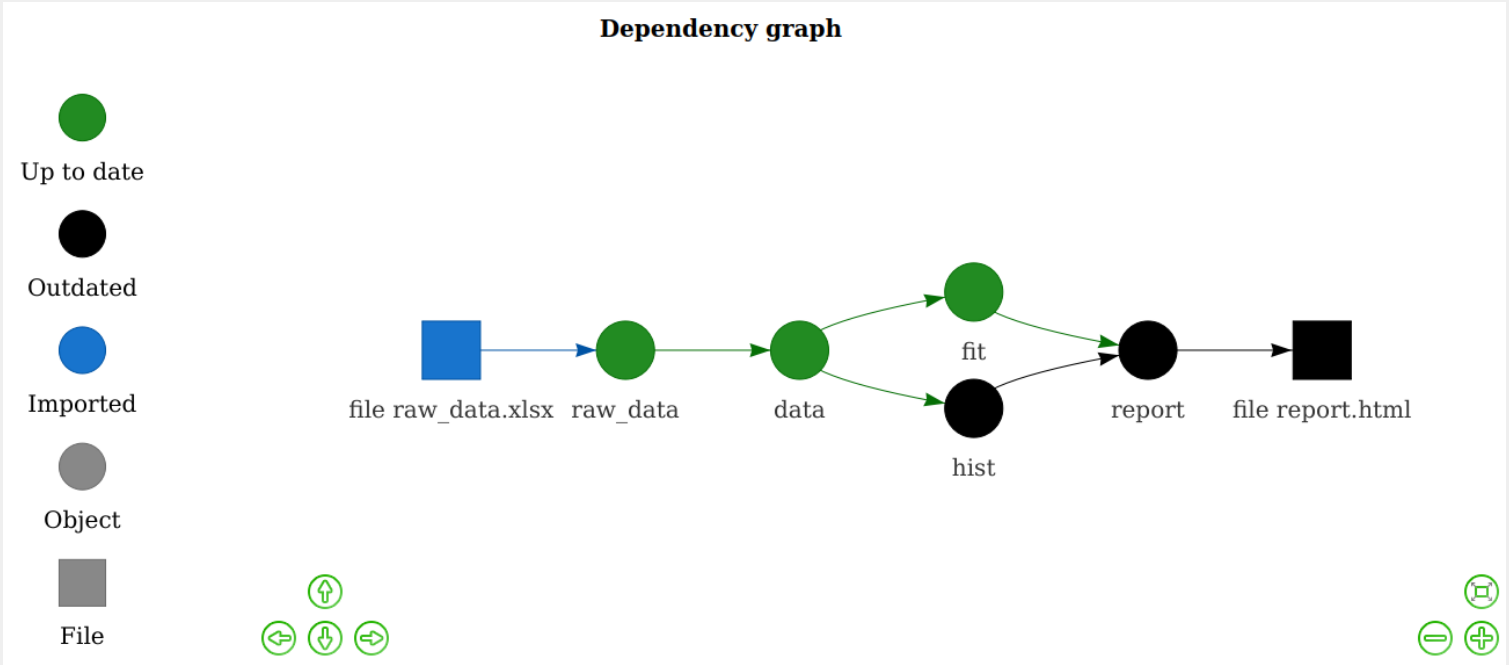
`make` for **R** projects.

GNU Make is a tool which controls the generation of executables and other non-source files of a program from the program's source files.

Source: GNU Make web page.

```
plan <- drake_plan(
  raw_data = read_excel(file_in("raw_data.xlsx")),
  data = raw_data %>%
    mutate(Species = fct_inorder(Species)),
  hist = create_plot(data),
  fit = lm(Sepal.Width ~ Petal.Width + Species, data),
  report = rmarkdown::render(
    knitr_in("report.Rmd"),
    output_file = file_out("report.html"),
    quiet = TRUE
  )
)
```

DRAKE


Dependency graph
Up to date
Outdated
Imported
Object
File
file raw_data.xlsx
raw_data
data
fit
hist
report
file report.html

Parallelization:

```
# multicore scaling
make(plan, jobs = 12)

# or enable supercomputing clusters with
# the future package
drake_hpc_template_file("torque_batchtools.tmpl")
library(future.batchtools)
future::plan(batchtools_torque,
             template = "torque_batchtools.tmpl",
             workers = 8000)
make(plan, parallelism = "future_lapply")
```

MI² Data Lab

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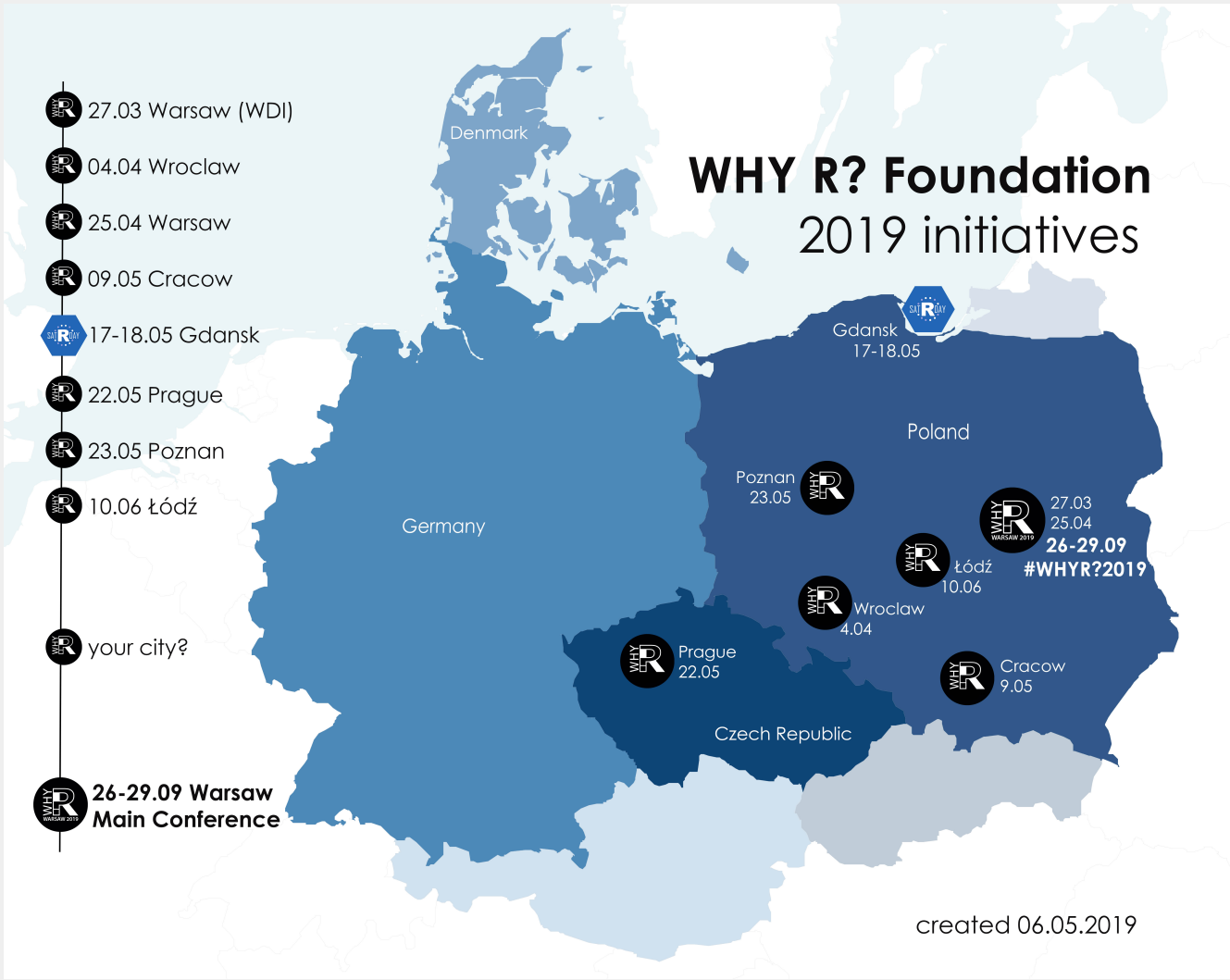
WHY R? 2019}


27.03 Warsaw (WDI)
04.04 Wroclaw
25.04 Warsaw
09.05 Cracow
17-18.05 Gdansk
22.05 Prague
23.05 Poznan
10.06 Łódź
your city?
26-29.09 Warsaw
Main Conference
Denmark
Germany
Poland
Czech Republic
WHY R? Foundation
2019 initiatives
Gdansk
17-18.05
Poznan
23.05
Łódź
10.06
Wroclaw
4.04
Prague
22.05
Cracow
9.05
27.03
25.04
26-29.09
#WHYR?2019
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