compboost

Fast and Flexible Component-Wise Boosting

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Use-Case

- We own a small booth at the Christmas market that sells mulled wine.

- As we are very interested in our customers' health, we only sell to customers who we expect to drink less than 15 liters per season.

- To estimate how much a customer drinks, we have collected data from 200 customers in recent years.

- These data include mulled wine consumption (in liter and cups), age, sex, country of origin, weight, body size, and 200 characteristics gained from app usage (that have absolutely no influence).

mw_consumption	mw_consumption_cups	gender	country	age	weight	height	app_usage1
12.6	42	f	Seychelles	21	119.25	157.9	0.1680
2.1	7	f	Poland	57	67.72	157.5	0.8075
12.6	42	m	Seychelles	25	65.54	181.6	0.3849
9.3	31	f	Germany	68	84.81	195.9	0.3277
4.8	16	m	Ireland	39	85.30	163.9	0.6021
9.3	31	f	Germany	19	102.75	173.8	0.6044
5.1	17	f	Poland	66	98.54	199.7	0.1246
7.5	25	f	Seychelles	62	108.21	198.1	0.2946
15.0	50	m	Seychelles	22	62.08	180.1	0.5776
8.4	28	m	Germany	52	75.42	170.0	0.6310

With these data we want to answer the following questions:

- Which of the customers' characteristics are important to be able to determine the consumption?

- How does the effect of important features look like?

- How does the model behave on unseen data?

What can we do to answer all the questions?

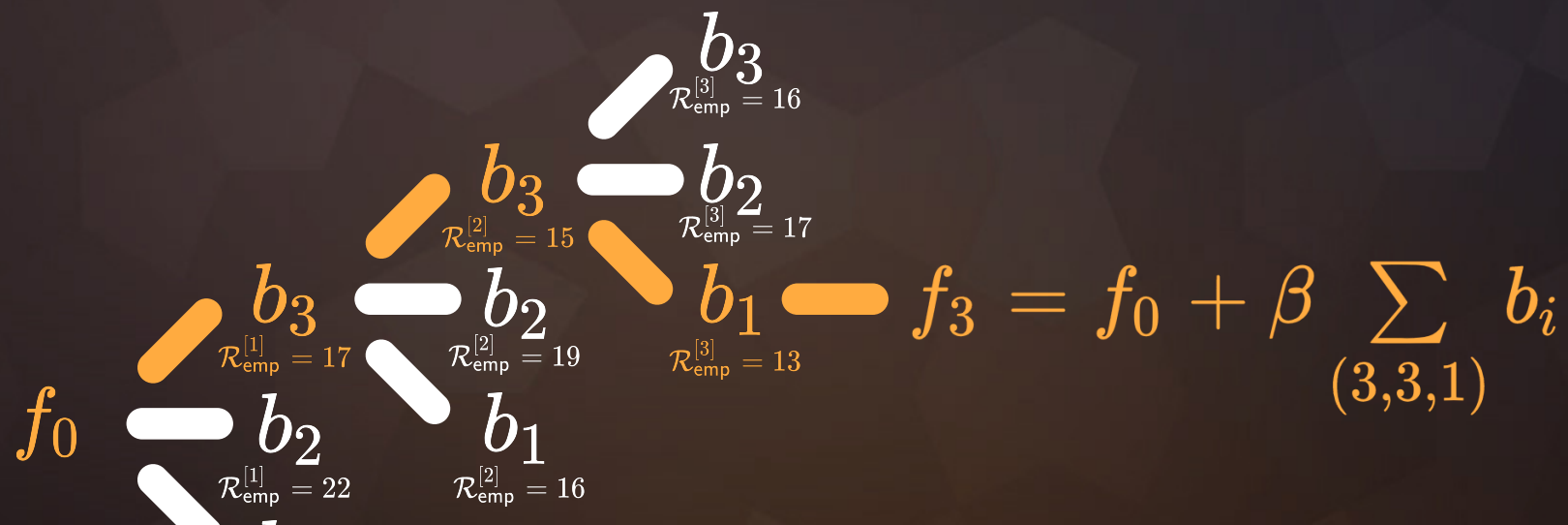**What can we do to answer all the questions?**

- Fit a linear model?

- Fit a linear model on each feature and build the ensemble?

- Fit a regularized linear model?

- Train a random forest?

What can we do to answer all the questions?

- Fit a linear model?
  $\longrightarrow$ Not possible since $p > n$.

- Fit a linear model on each feature and build the ensemble?
  $\longrightarrow$ Possible, but how should we determine important effects?

- Fit a regularized linear model?
  $\longrightarrow$ Possible, but with the linear model we get just linear effects.

- Train a random forest?
  $\longrightarrow$ Possible, but we want to interpret the effects.

Component-Wise Boosting

b_3
$\mathcal{R}_{\text{emp}}^{[3]} = 16$

b_3
$\mathcal{R}_{\text{emp}}^{[2]} = 15$

b_2
$\mathcal{R}_{\text{emp}}^{[3]} = 17$

b_3
$\mathcal{R}_{\text{emp}}^{[1]} = 17$

b_2
$\mathcal{R}_{\text{emp}}^{[2]} = 19$

b_1
$\mathcal{R}_{\text{emp}}^{[3]} = 13$

$$f_3 = f_0 + \beta \sum_{(3,3,1)} b_i$$

f_0

b_2
$\mathcal{R}_{\text{emp}}^{[1]} = 22$

b_1
$\mathcal{R}_{\text{emp}}^{[2]} = 16$

Why Component-Wise Boosting?

- Inherent (unbiased) feature selection.

- Resulting model is sparse since important effects are selected first and therefore it is able to learn in high-dimensional feature spaces ($p \gg n$).

- Parameters are updated iteratively. Therefore, the whole trace of how the model evolves is available.

About `compboost`

The `compboost` package is a fast and flexible framework for model-based boosting completely written in `C++`:

- With `mboost` as standard, we want to keep the modular principle of defining custom base-learner and losses.

- Completely written in `C++` and exposed by `Rcpp` to obtain high performance and full memory control.

- `R` API is written in `R6` to provide convenient wrapper.

- Major parts of the `compboost` functionality are unit tested against `mboost` to ensure correctness.

Applying compboost to the Use-Case

Quick Start With Wrapper Functions

```r
cboost = boostSplines(data = mulled_wine_data[,-2],
  target = "mw_consumption", loss = LossQuadratic$new(),
  learning.rate = 0.005, iterations = 6000, trace = 600)
##     1/6000   risk = 5.6
##   600/6000   risk = 2.5
## 1200/6000   risk = 1.3
## 1800/6000   risk = 0.8
## 2400/6000   risk = 0.51
## 3000/6000   risk = 0.34
## 3600/6000   risk = 0.24
## 4200/6000   risk = 0.17
## 4800/6000   risk = 0.12
## 5400/6000   risk = 0.087
## 6000/6000   risk = 0.064
##
##
## Train 6000 iterations in 8 Seconds.
## Final risk based on the train set: 0.064
```

Effect Visualization

```
cboost$plot("age_spline", iters = c(200, 500, 1000, 3000))
```

Effect of age_spline
Additive contribution of predictor
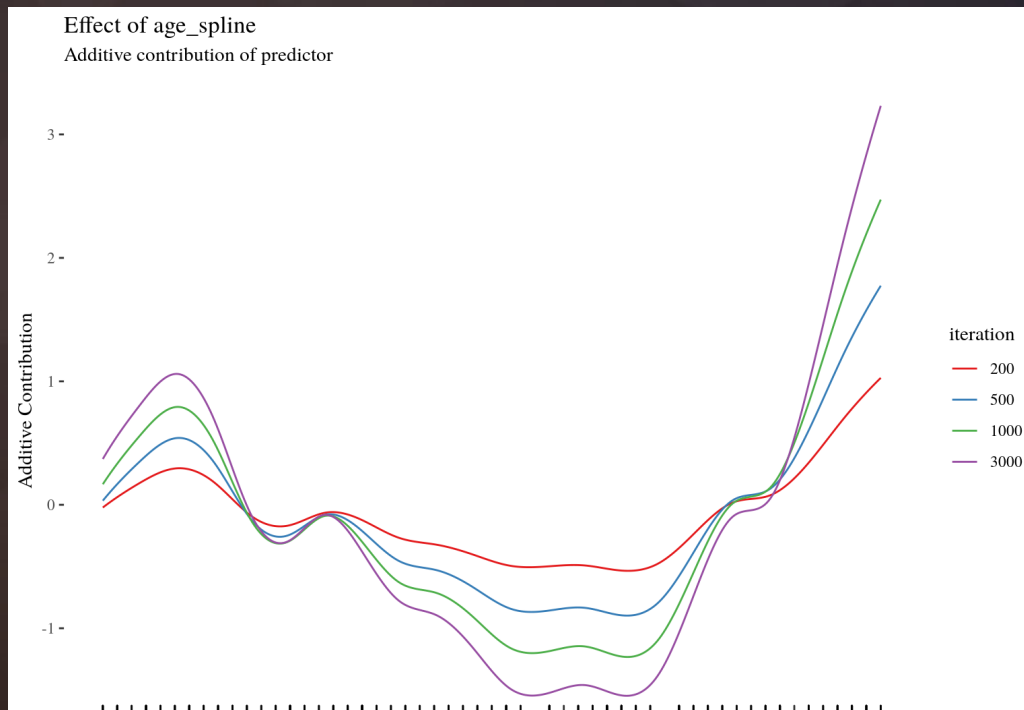
Inbag and OOB Behavior

To get an idea, how the model behaves on unseen data we use 75 % as training data and the other 25 % of the data to calculate the out of bag (OOB) risk:

```r
n_data = nrow(mulled_wine_data)
idx_train = sample(x = seq_len(n_data), size = n_data * 0.75)
idx_test = setdiff(x = seq_len(n_data), idx_train)
```

Define Model and Base-Learner the "Object-Oriented Style"

```r
cboost = Compboost$new(data = mulled_wine_data[idx_train,-2],
  target = "mw_consumption", loss = LossQuadratic$new(),
  learning.rate = 0.005)

target_vars = c("mw_consumption", "mw_consumption_cups")

for (feature_name in setdiff(names(mulled_wine_data), target_vars)) {

  if (feature_name %in% c("gender", "country")) {
    cboost$addBaselearner(feature = feature_name, id = "category",
      bl.factory = BaselearnerPolynomial, intercept = FALSE)
  } else {
    cboost$addBaselearner(feature = feature_name, id = "spline",
      bl.factory = BaselearnerPSpline, degree = 3, n.knots = 10)
  }
}
```

OOB Data

To track the OOB risk we have to prepare the new data so that `compboost` knows the new data sources:

```
oob_data = cboost$prepareData(mulled_wine_data[idx_test,])
oob_response = mulled_wine_data$mw_consumption[idx_test]
```

Define Logger

```r
cboost$addLogger(logger = LoggerOobRisk, logger.id = "oob_risk",
  used.loss = LossQuadratic$new(), eps.for.break = 0,
  oob.data = oob_data, oob.response = oob_response)

cboost$addLogger(logger = LoggerTime, logger.id = "microseconds",
  max.time = 0, time.unit = "microseconds")

cboost$train(6000, trace = 1500)

##    1/6000   risk = 5.6   microseconds = 1      oob_risk = 5.7
## 1500/6000   risk = 0.99  microseconds = 2348546   oob_risk = 1.5
## 3000/6000   risk = 0.37  microseconds = 4687547   oob_risk = 1.1
## 4500/6000   risk = 0.17  microseconds = 7082161   oob_risk = 1.1
## 6000/6000   risk = 0.092 microseconds = 9418308   oob_risk = 1.2
##
##
## Train 6000 iterations in 9 Seconds.
## Final risk based on the train set: 0.092
```

Extract Inbag and OOB Data

```r
inbag_trace = cboost$getInbagRisk()
head(inbag_trace)
## [1] 5.659 5.647 5.635 5.623 5.612 5.600


logger_data = cboost$getLoggerData()
head(logger_data)

##   _iterations microseconds oob_risk
## 1           1            1    5.671
## 2           2         1639    5.660
## 3           3         3216    5.649
## 4           4         4827    5.639
## 5           5         6390    5.628
## 6           6         7986    5.618
```

Visualization of Inbag and OOB Risk

```r
oob_trace = logger_data[["oob_risk"]]

risk_data = data.frame(
  risk = c(inbag_trace, oob_trace),
  type = rep(c("inbag", "oob"), times = c(length(inbag_trace),
    length(oob_trace))),
  iter = c(seq_along(inbag_trace), seq_along(oob_trace))
)
ggplot(risk_data, aes(x = iter, y = risk, color = type)) + geom_line()
```
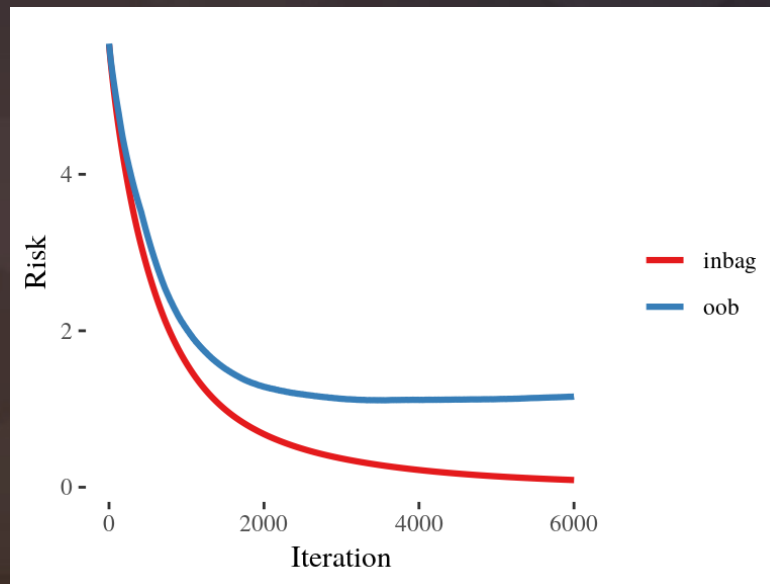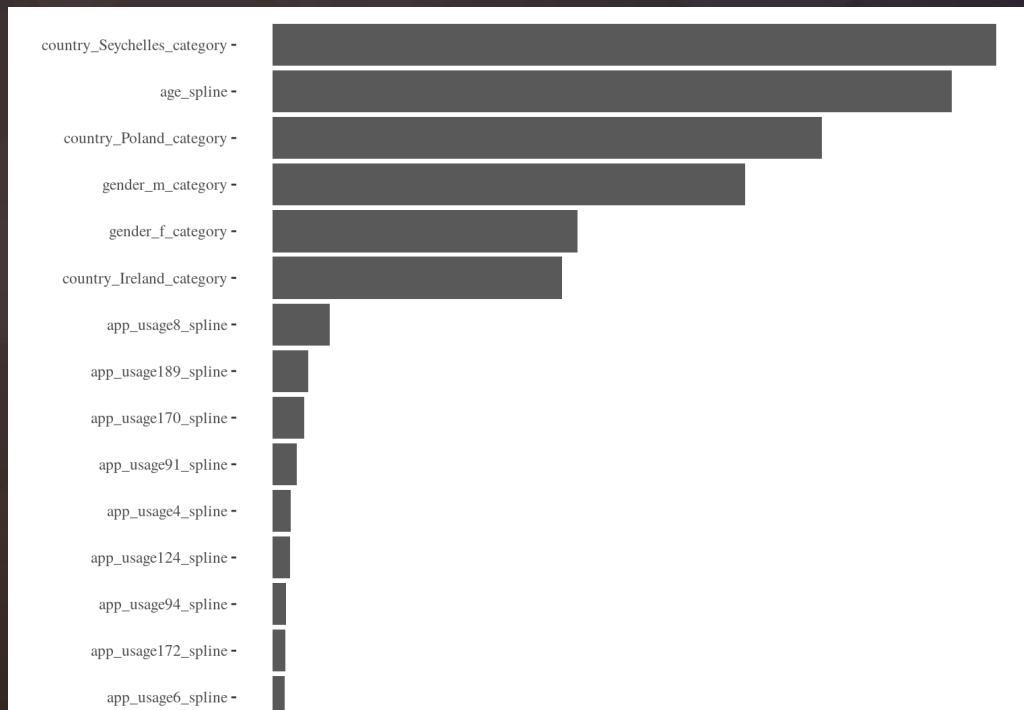
Set Model to a Specific Iteration

```
cboost$train(2200)
cboost
## Component-Wise Gradient Boosting
##
## Trained on mulled_wine_data[idx_train, -2] with target mw_consumption
## Number of base-learners: 210
## Learning rate: 0.005

## Iterations: 2200
## Offset: 6.65
##
## LossQuadratic Loss:
##
##    Loss function: L(y,x) = 0.5 * (y - f(x))^2
##
##
```

Feature Importance

```
cboost$plotFeatureImportance(num.feat = 15L)
```

Using Custom Losses - Defining a Loss

As customers do not buy the wine in liters but per cup, it might be better to use a Poisson loss to take the counting data into account. For that reason we define a custom loss:

```r
lossPoi = function (truth, pred) {
  return (-log(exp(pred)^truth * exp(-exp(pred)) / gamma(truth + 1)))

}
gradPoi = function (truth, pred) {
  return (exp(pred) - truth)
}
constInitPoi = function (truth) {
  return (log(mean.default(truth)))
}
# Define custom loss:
my_custom_loss = LossCustom$new(lossPoi, gradPoi, constInitPoi)
```

Using Custom Losses - Using the Loss

```r
cboost = boostSplines(data = mulled_wine_data[,-1],
  target = "mw_consumption_cups", loss = my_custom_loss,
  optimizer = OptimizerCoordinateDescent$new(),
  learning.rate = 0.005, iterations = 500, trace = 100,
  n.knots = 10, degree = 3)
##    1/500    risk = 5.3
## 100/500    risk = 3

## 200/500    risk = 2.7
## 300/500    risk = 2.6
## 400/500    risk = 2.6
## 500/500    risk = 2.5
##
##
## Train 500 iterations in 0 Seconds.
## Final risk based on the train set: 2.5
```

Further Functionalities

- Each logger can also be used as stopper, therefore we can use them for early stopping

- In combination with the custom loss, we can use the OOB logger to track performance measures like the AUC (in binary classification)

- Losses and base-learner can also be directly extended using `C++` (see `getCustomCppExample()`)

From C++ to R

Rcpp

- Automated conversion between `R` and `C++` data structures, such as vectors, matrices, or even whole classes

- Seamless integration of Armadillo for linear algebra

- Complicated stuff like compilation, or again, the conversion between `R` and `C++` are handled automatically

C++ to R Wrap Up of `compboost`

R

```
> cboost = Compboost$new(...)
```

```
> cboost$addBaselearner(feat)
```

```
> cboost$addLogger(logger)
```

C++

```
> bl_list = BaselearnerFactoryList(...)
> l_list  = LoggerList(...)
> loss    = new LossQuadratic(...)
> optim   = new OptimizerCoordinateDesc(...)
```

```
> source = InMemoryData(feat)
> target = InMemoryData()
> bl_feat = BaselearnerPSpline(source, target)
> bl_list.registerBaselearner(bl_feat)
```

```
> logger = LoggerOOBRisk(...)
> l_list.registerLogger(logger)
```

Challenges When Using C++ and Rcpp

- Saving object is not possible at the moment

- Memory managing is not easy $\Rightarrow$ Segmentation folds or memory leaks may happen

- Exported API of classes is not very informative

- Debugging of `C++` from `R` can be very annoying and time-consuming

What's Next?

- Better selection process of base-learner

- Speed up the training by parallel computations

- Greater functionality:

  - Functional data structures and loss functions

  - Unbiased feature selection

  - Effect decomposition into constant, linear, and non-linear

Thanks for your attention!

build passing   build passing   coverage 97%   license MIT   CRAN 0.1.0   JOSS 10.21105/joss.00967
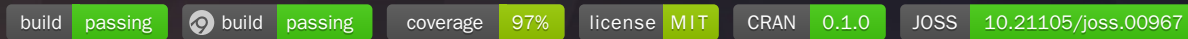
Actively developed on GitHub:

https://github.com/schalkdaniel/compboost

Project page:

https://compboost.org/

Credits

Slides were created with:

- revealjs

- Font-Awesome:

- rmarkdown

- revealjs (R Package)

- Google Fonts