The big picture

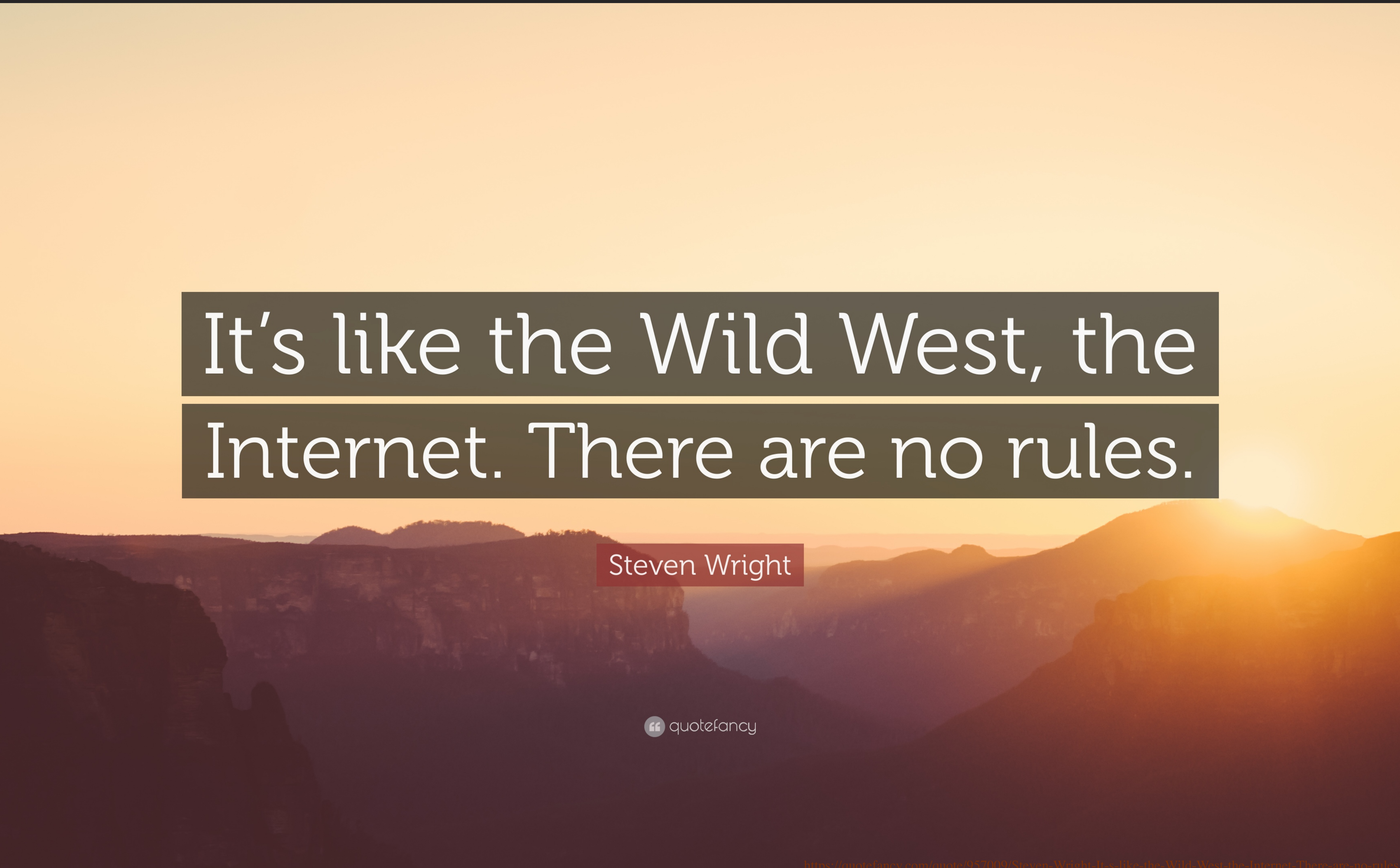
useR - July 2019

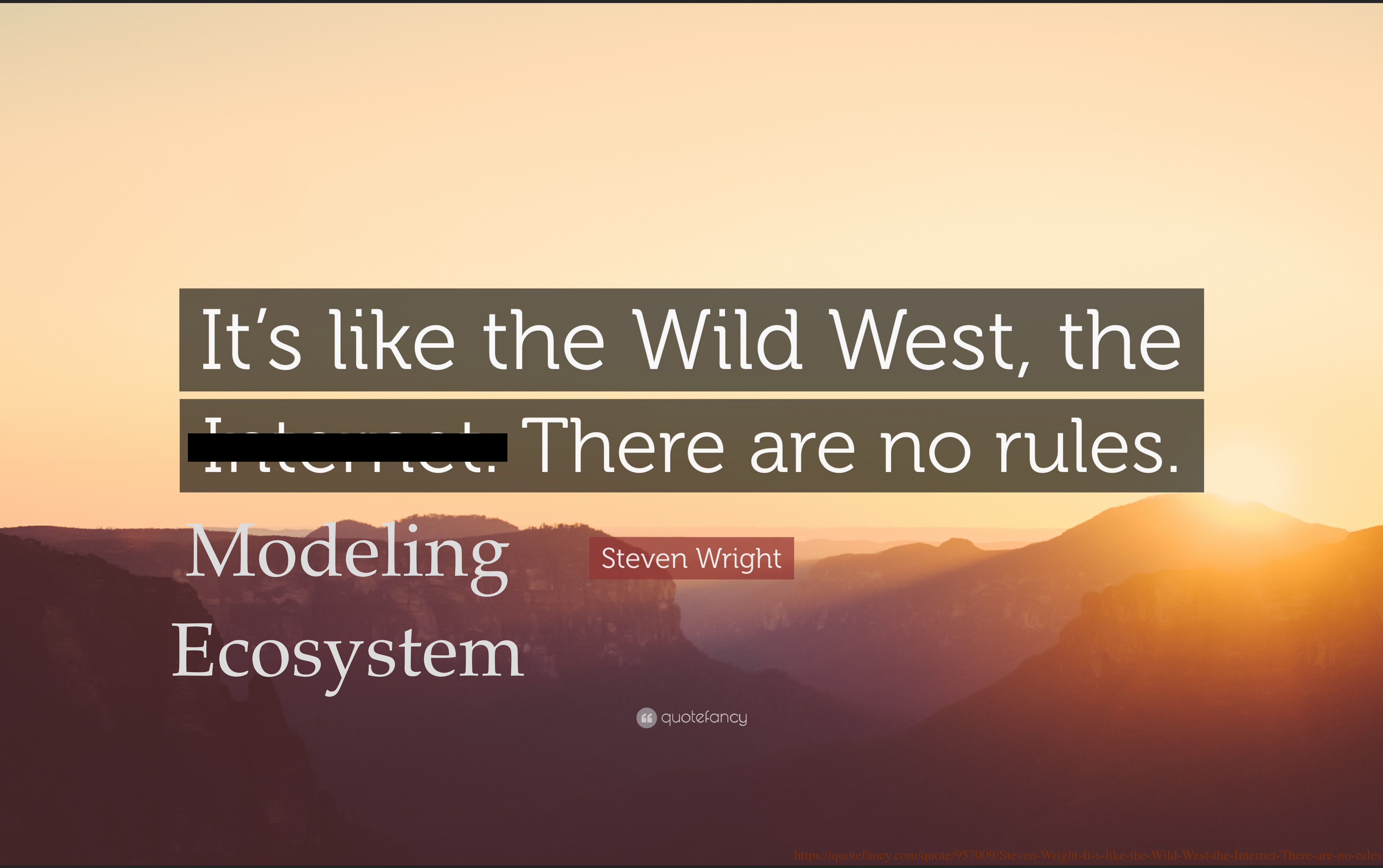
RStudio

The modeling ecosystem

Case study

The R Modeling Ecosystem


It’s like the Wild West, the Internet. There are no rules.
Steven Wright
quotefancy
https://quotefancy.com/quote/957009/Steven-Wright-It-s-like-the-Wild-West-the-Internet-There-are-no-rules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[redacted] There are no rules.
Steven Wright
Modeling
Ecosystem
quotefancy

But I thought R was good at modeling?

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It is.

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It is.

But…

A problem of consistency

Function	**Package**	**Code**
`lda`	`MASS`	`predict(obj)`
`glm`	`stats`	`predict(obj, type = "response")`
`gbm`	`gbm`	`predict(obj, type = "response", n.trees)`
`mda`	`mda`	`predict(obj, type = "posterior")`
`rpart`	`rpart`	`predict(obj, type = "prob")`
`Weka`	`RWeka`	`predict(obj, type = "probability")`
`logitboost`	`LogitBoost`	`predict(obj, type = "raw", nIter)`
`pamr.train`	`pamr`	`pamr.predict(obj, type = "posterior", threshold)`

A problem of consistency

Function	Package	Code
[illegible]	MASS	predict(obj)
[illegible]	[illegible]	predict(obj, type = "response")
gbm	[illegible]	[illegible] type = "response", n.trees)
mda	mda	[illegible]ior")
rpart	rpart	predict(obj, [illegible]
Weka	RWeka	predict(obj, type = "probabi[illegible]
logitboost	LogitBoost	predict(obj, type = "raw", nIter)
pamr.train	pamr	pamr.predict(obj, type = "posterior", threshold)

predict(obj, type = “prob”)

tidymodels

```r
library(parsnip)
train <- mtcars[1:20,]
test <- mtcars[21:32,]
```

```r
linear_reg(penalty = .01) %>%
  set_engine("glmnet") %>%
  fit(mpg ~ cyl + disp, train) %>%
  predict(test)
#> # A tibble: 12 x 1
#>    .pred
#>    <dbl>
#>  1  26.5
#>  2  15.1
#>  3  15.5
#>  4  14.4
#>  5  13.2
#>  6  27.5
#>  7  26.5
#>  8  27.1
#>  9  14.4
#> 10  22.6
#> 11  15.6
#> 12  26.5
```

```r
rand_forest(mode = "regression") %>%
  set_engine("ranger") %>%
  fit(mpg ~ cyl + disp, train) %>%
  predict(test)
#> # A tibble: 12 x 1
#>    .pred
#>    <dbl>
#>  1  25.0
#>  2  15.6
#>  3  15.7
#>  4  15.6
#>  5  15.5
#>  6  30.2
#>  7  25.0
#>  8  26.7
#>  9  15.6
#> 10  21.5
#> 11  15.7
#> 12  25.0
```

Lets talk about xgboost

Lets talk about xgboost

Gradient boosting is a machine learning technique for regression and classification problems, which produces a prediction model in the form of an ensemble of weak prediction models, typically decision trees.

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https://en.wikipedia.org/wiki/Gradient_boosting

Lets talk about xgboost

Lets talk about
xgboost

Written by C developers as an R
interface to a C library

```r
library(xgboost)
library(dplyr)

outcome <- pull(iris, Species)
predictors <- select(iris, -Species)

head(outcome)
#> [1] setosa setosa setosa setosa setosa setosa
#> Levels: setosa versicolor virginica

head(predictors)
#>   Sepal.Length Sepal.Width Petal.Length Petal.Width
#> 1          5.1         3.5          1.4         0.2
#> 2          4.9         3.0          1.4         0.2
#> 3          4.7         3.2          1.3         0.2
#> 4          4.6         3.1          1.5         0.2
#> 5          5.0         3.6          1.4         0.2
#> 6          5.4         3.9          1.7         0.4
```

```r
model ← xgboost(
  data      = predictors,
  label     = outcome,
  objective = "multi:softprob"
)
```

```r
model <- xgboost(
  data      = predictors,
  label     = outcome,
  objective = "multi:softprob"
)

#> Warning in xgb.get.DMatrix(data, label, missing,
#> weight): xgboost: label will be ignored.

#> Error in xgb.get.DMatrix(data, label, missing,
#> weight): xgboost doesn't support data.frame as
#> input. Convert it to matrix first.
```

```r
model ← xgboost(
  data      = as.matrix(predictors),
  label     = outcome,
  objective = "multi:softprob"
)
```

```r
model <- xgboost(
  data      = as.matrix(predictors),
  label     = outcome,
  objective = "multi:softprob"
)

#> Error in check.booster.params(params, ...):
#> 'num_class' > 1 parameter must be set for
#> multiclass classification
```

```r
model <- xgboost(
  data      = as.matrix(predictors),
  label     = outcome,
  objective = "multi:softprob"
)

#> Error in check.booster.params(params, ...):
#> 'num_class' > 1 parameter must be set for
#> multiclass classification
```

num_class set the number of classes.
To use only with multiclass objectives.

```r
model <- xgboost(
  data      = as.matrix(predictors),
  label     = outcome,
  objective = "multi:softprob",
  num_class = 3
)
```

```r
model <- xgboost(
  data      = as.matrix(predictors),
  label     = outcome,
  objective = "multi:softprob",
  num_class = 3
)

#> Error in xgb.train(params, dtrain, nrounds,
#> watchlist, verbose = verbose, :
#> argument "nrounds" is missing, with no default
```

```r
model <- xgboost(
  data      = as.matrix(predictors),
  label     = outcome,
  objective = "multi:softprob",
  num_class = 3,
  nrounds   = 10
)
```

```r
model <- xgboost(
  data      = as.matrix(predictors),
  label     = outcome,
  objective = "multi:softprob",
  num_class = 3,
  nrounds   = 10
)

#> Error in xgb.iter.update(bst$handle, dtrain,
#> iteration - 1, obj): [12:15:39] amalgamation/../
#> src/objective multiclass_obj.cu:110:
#> SoftmaxMultiClassObj: label must be in
#> [0, num_class).
#>
#> Stack trace returned 10 entries:
#> [bt] (0) 0   xgboost.so
#> 0x000000010f7bb23c dmlc::StackTrace(unsigned long)
#> + 460
#> ..BLAHHHHHHH
```

```r
model <- xgboost(
  data        = as.matrix(predictors),
  label       = outcome,
  objective = "multi:softprob",
  num_class = 3,
  nrounds   = 10
)

#> Error in xgb.iter.update(bst$handle, dtrain,
#> iteration - 1, obj): [12:15:39] amalgamation/../
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#> SoftmaxMultiClassObj: label must be in
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#> 0x000000010f7bb23c dmlc::StackTrace(unsigned long)
#> + 460
#>  ..BLAHHHHHHH
```

```r
model <- xgboost(
  data      = as.matrix(predictors),
  label     = as.numeric(outcome) - 1L,
  objective = "multi:softprob",
  num_class = 3,
  nrounds   = 10
)

#> [1]  train-merror:0.020000
#> [2]  train-merror:0.026667
#> [3]  train-merror:0.020000
#> [4]  train-merror:0.020000
#> [5]  train-merror:0.013333
#> [6]  train-merror:0.013333
#> [7]  train-merror:0.013333
#> [8]  train-merror:0.013333
#> [9]  train-merror:0.013333
#> [10] train-merror:0.013333
```

Constructive feedback 🤔

Why can’t predictors be a data frame?

Why force me to specify num_class?

Why do I always have to set nrounds?

Why can’t outcome be a factor?

Why does outcome have to be a 0-based integer?

Constructive feedback 🤔

Why can’t predictors be a data frame?
Principle: Familiar interface

Why force me to specify num_class?
Principle: Good defaults

Why do I always have to set nrounds?
Principle: Good defaults

Why can’t outcome be a factor?
Principle: Familiar interface

Why does outcome have to be a 0-based integer?
Principle: Familiar interface

```r
predict(model, as.matrix(predictors))

#>   [1] 0.95302665 0.02447842 0.02249493 0.95302665 0.02447842
#>   [6] 0.95302665 0.02447842 0.02249493 0.95302665 0.02447842
#>    ...
```

```r
predict(model, as.matrix(predictors))

#>   [1] 0.95302665 0.02447842 0.02249493 0.95302665 0.02447842
#>   [6] 0.95302665 0.02447842 0.02249493 0.95302665 0.02447842
#>    ...


0.95302665 + 0.02447842 + 0.02249493
#> [1] 1
```

```r
# Or `predict(model, as.matrix(predictors), reshape = TRUE)`
matrix(predict(model, as.matrix(predictors)), ncol = 3)

#>                 [,1]       [,2]       [,3]
#>   [1,] 0.95302665 0.02447842 0.02249493
#>   [2,] 0.95302665 0.02447842 0.02249493
#>   [3,] 0.95302665 0.02447842 0.02249493
#>   [4,] 0.95302665 0.02447842 0.02249493
#>    ..   ..   ..   ..
```

Constructive feedback 🤔

Why can't newdata be a data frame?
Principle: Familiar interface

Why is the default multiclass prob output a vector?
Principle: Predictable output

Note: If factors were allowed, the column names of the output could actually be meaningful!
Principle: User burden

In summary:

“I feel like I’m working for xgboost rather than having xgboost work for me.”

What makes a
modeling package “good”?

What makes a
modeling package “~~good~~”?
intuitive to use

Intuitive modeling packages:

Familiar interfaces

Good defaults

Familiar output types

Standardized arguments

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https://tidymodels.github.io/model-implementation-principles/

Intuitive modeling packages:

Think about the R <u>interface</u> in addition to the <u>implementation</u>

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Think about the R <ins>interface</ins> in addition to the <ins>implementation</ins>

Why doesn’t everyone do this?

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High barrier of
required knowledge

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High barrier of required knowledge

Low amount of tooling

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hardhat

“A toolkit for the construction of modeling packages”

- Opinionated
- Handles preprocessing
- Robust at prediction time
- S3 method advice
- Validation