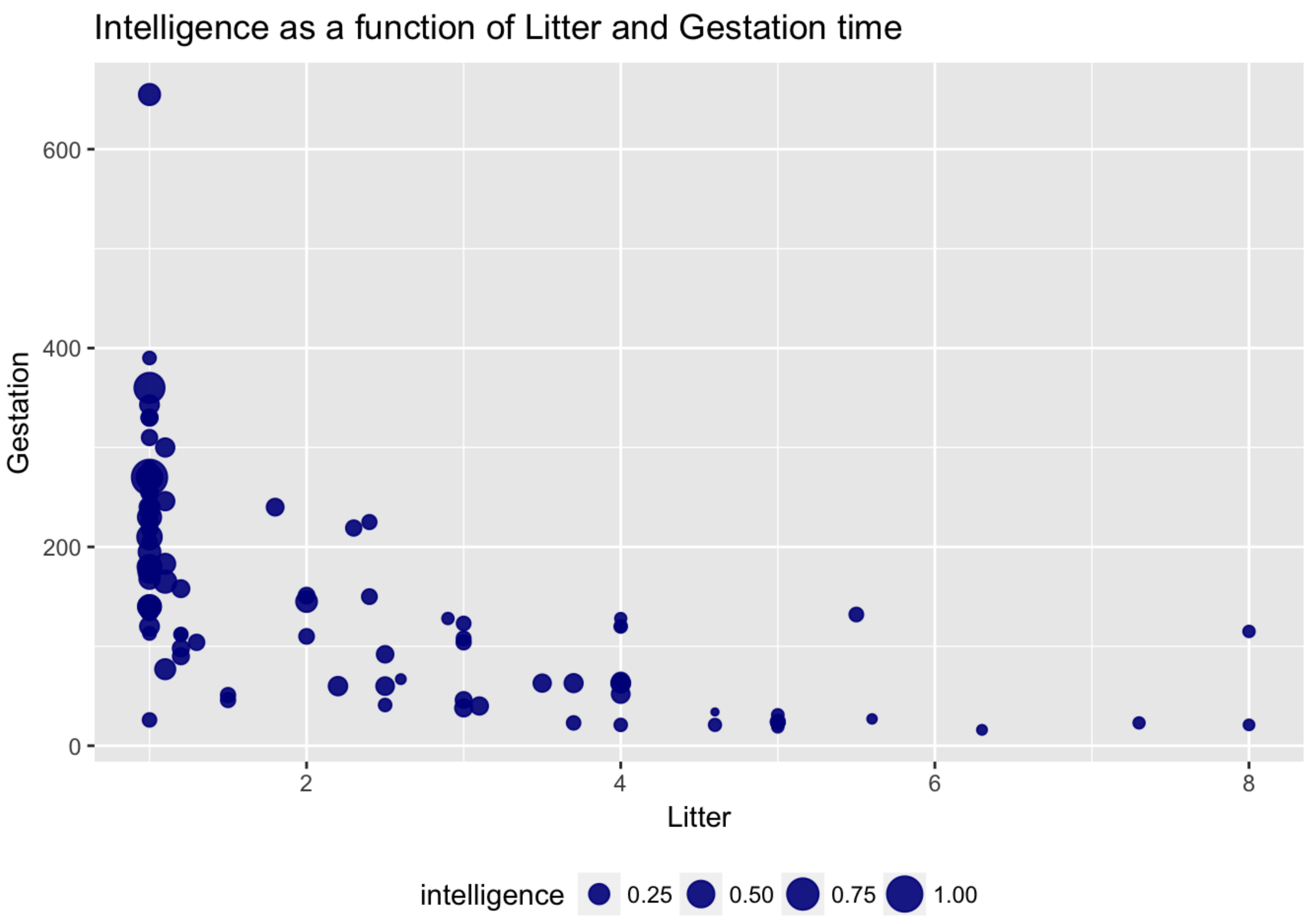
The intuition behind tree-based methods

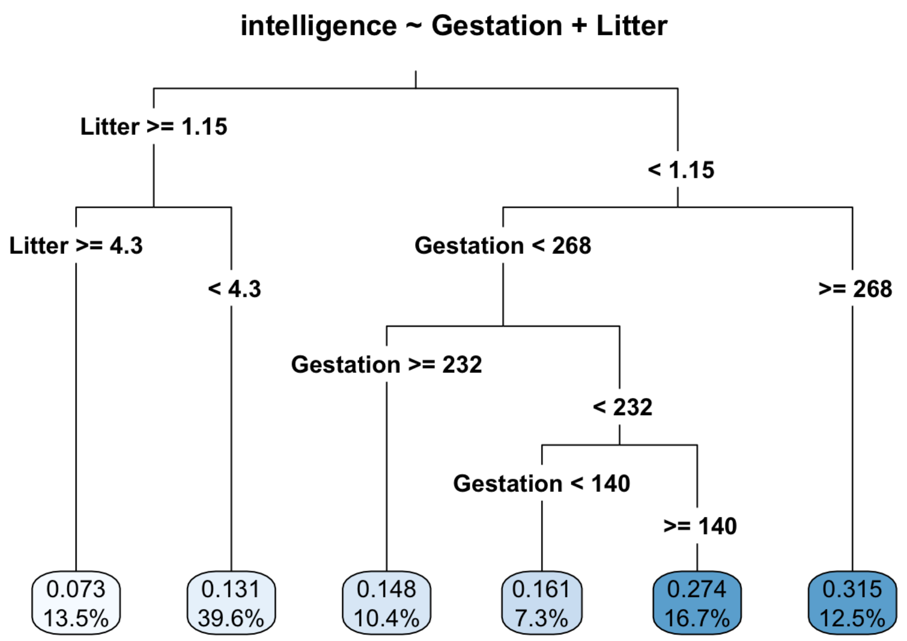
SUPERVISED LEARNING IN R: REGRESSION

Nina Zumel and John Mount
Win-Vector, LLC

Example: Predict animal intelligence from Gestation Time and Litter Size



Decision Trees



Rules of the form:

- *if a AND b AND c THEN y*

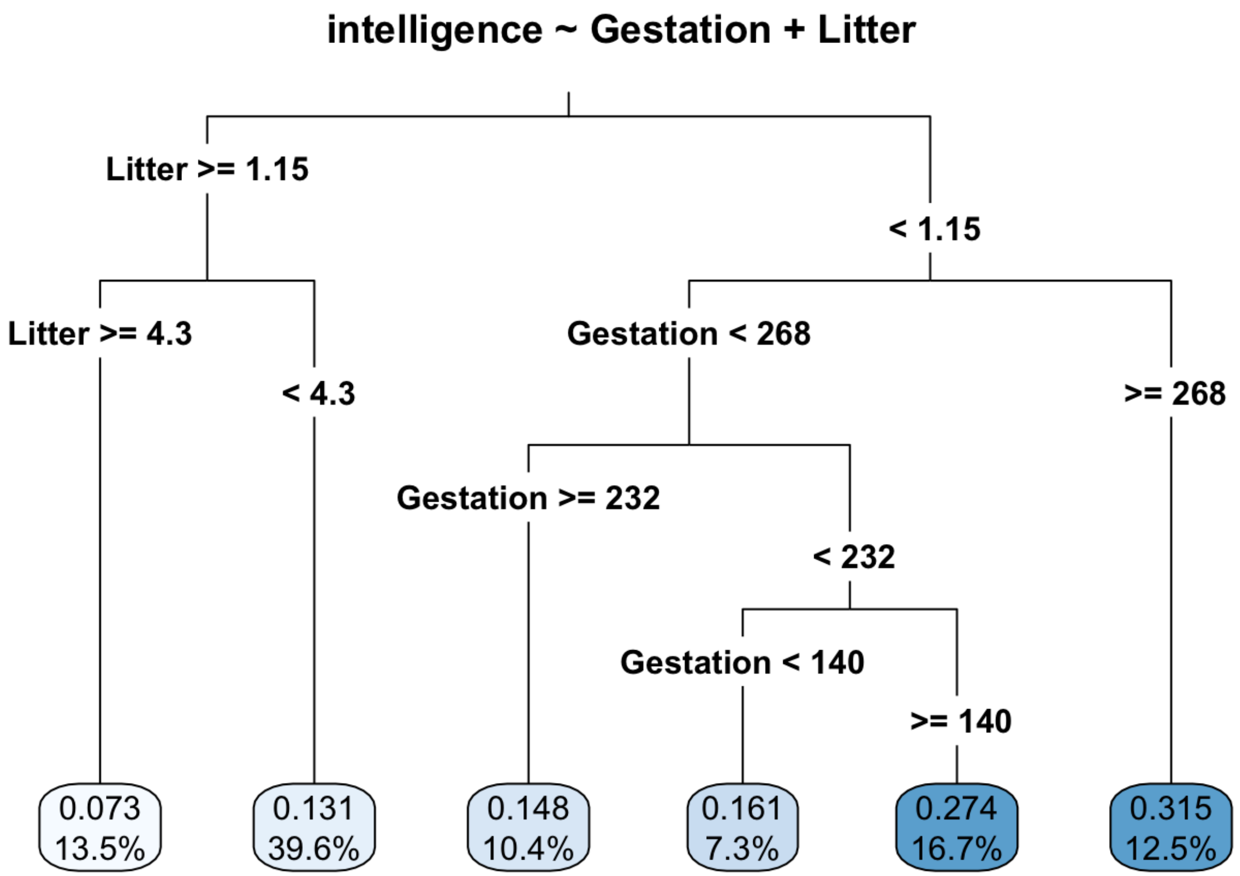
Non-linear concepts

- intervals
- non-monotonic relationships

non-additive interactions

- AND: similar to multiplication

Decision Trees



- IF Litter < 1.15 AND Gestation $\geq$ 268 $\rightarrow$ intelligence = 0.315
- IF Litter IN [1.15, 4.3) $\rightarrow$ intelligence = 0.131

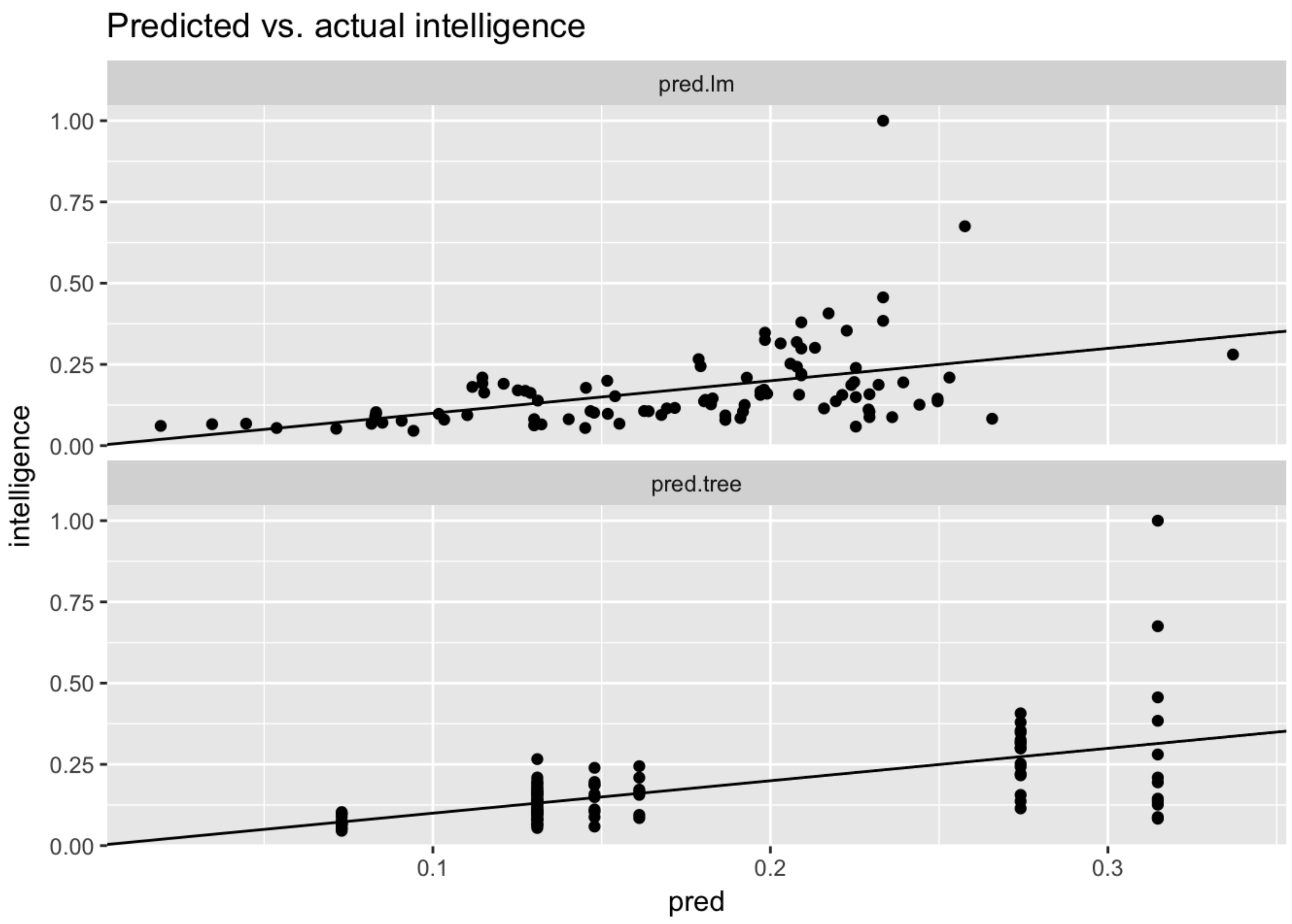
Decision Trees

Pro: Trees Have an *Expressive Concept Space*

Model	RMSE
linear	0.1200419
tree	0.1072732

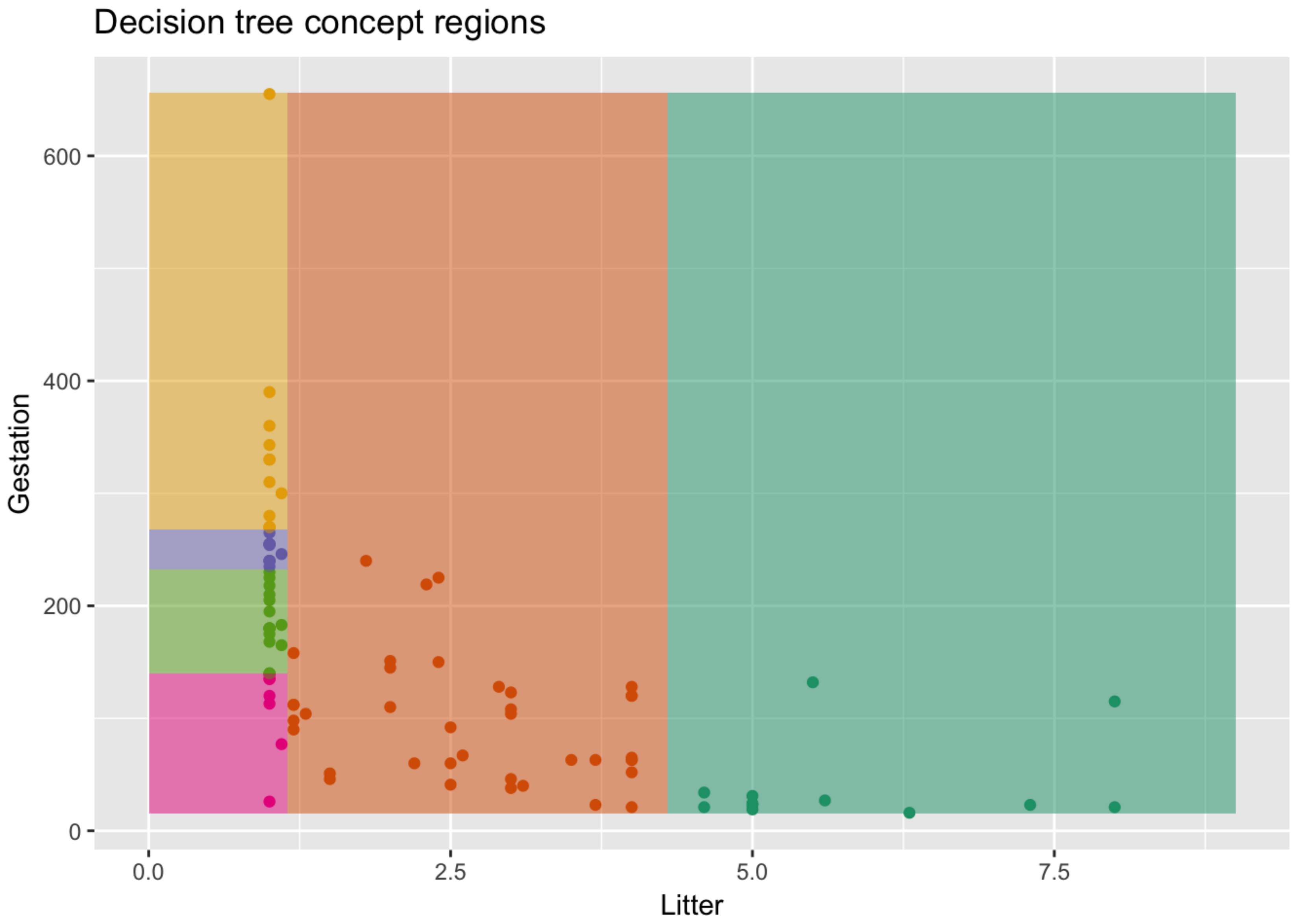
Decision Trees

Con: *Coarse-Grained Predictions*



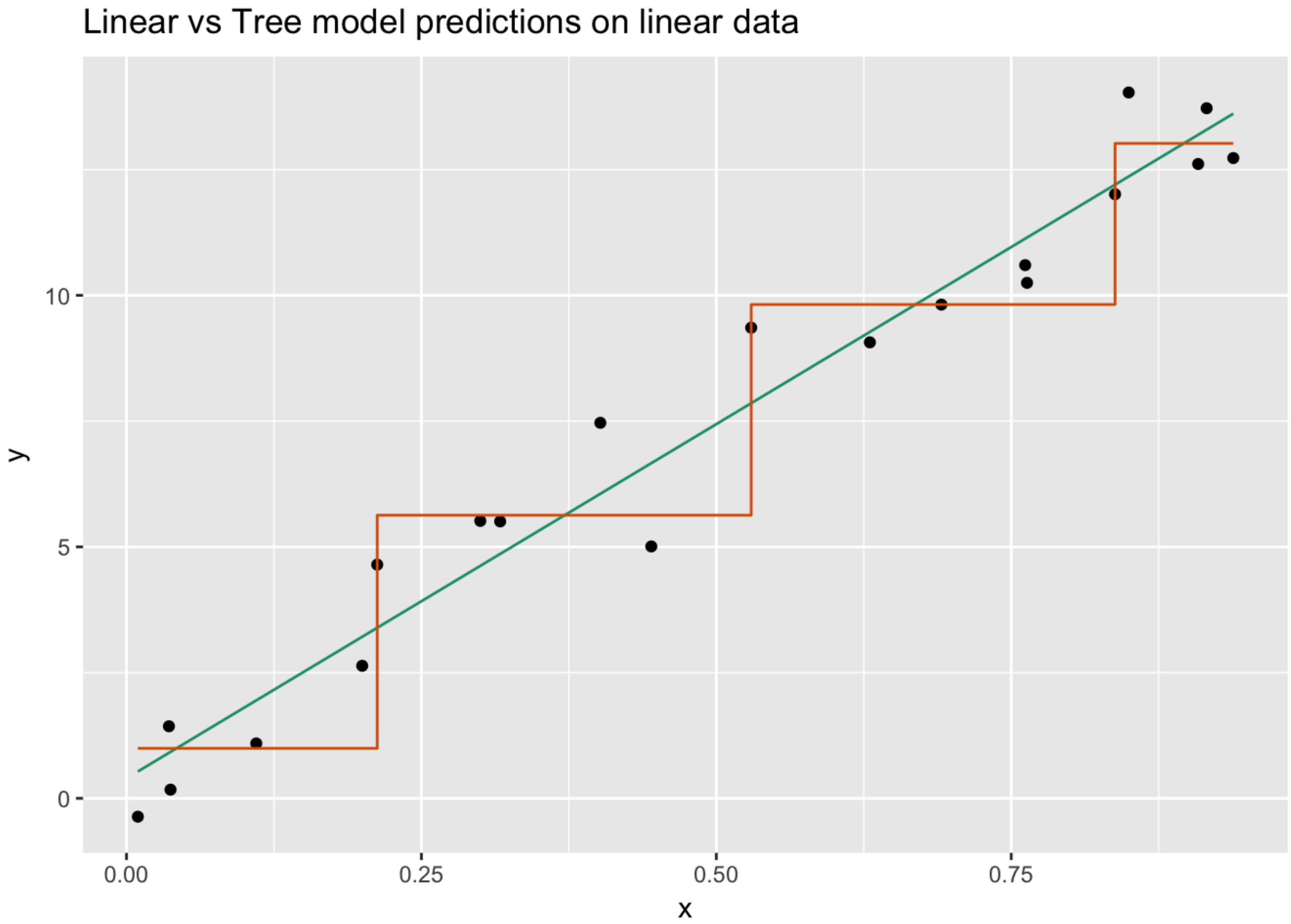
It's Hard for Trees to Express Linear Relationships

Trees Predict Axis-Aligned Regions



It's Hard for Trees to Express Linear Relationships

It's Hard to Express Lines with Steps

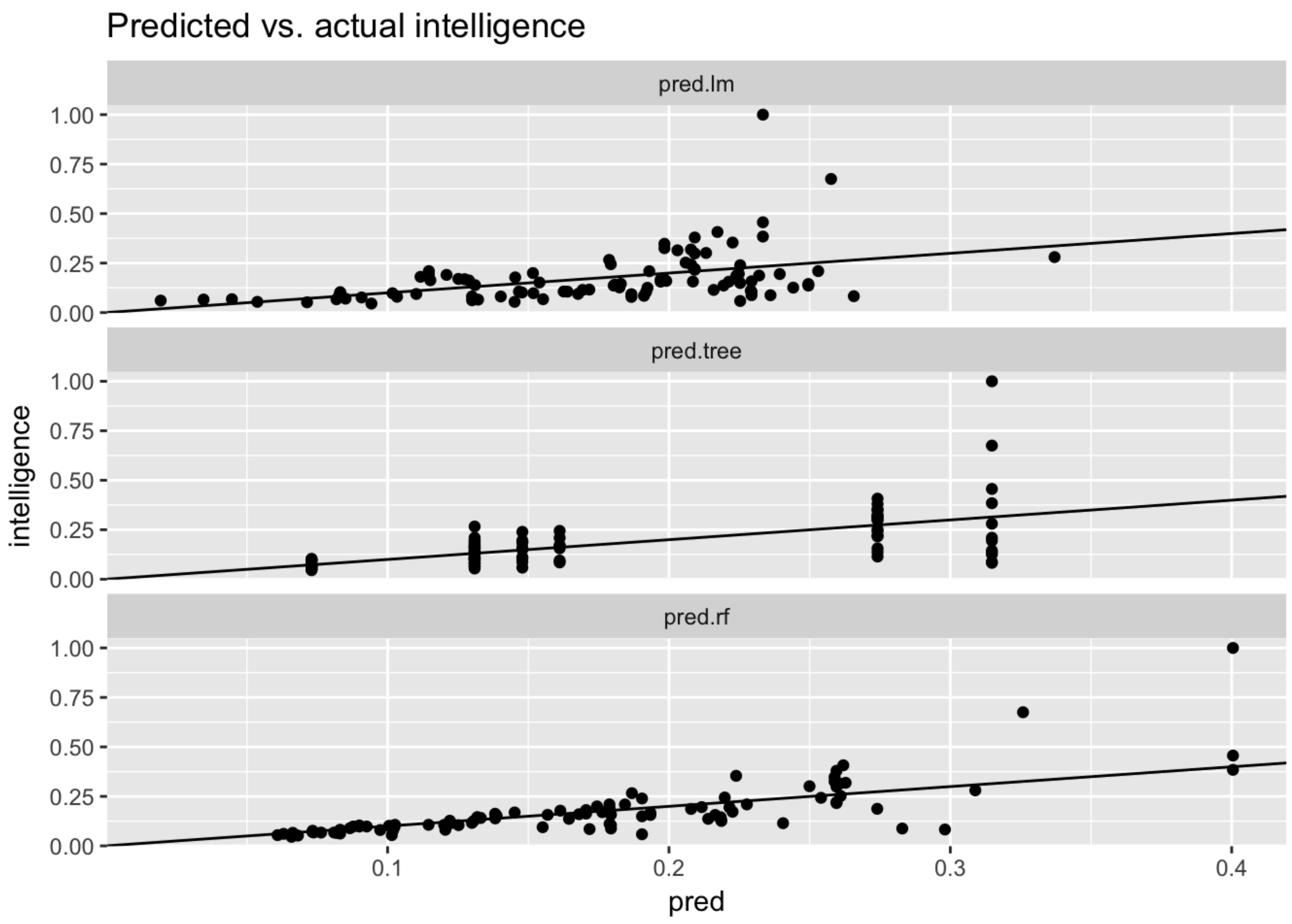


Other Issues with Trees

- Tree with too many splits (deep tree):
  - Too complex - danger of overfit
- Tree with too few splits (shallow tree):
  - Predictions too coarse-grained

Ensembles of Trees

Ensembles Give Finer-grained Predictions than Single Trees



Ensembles of Trees

Ensemble Model Fits Animal Intelligence Data Better than Single Tree

Model	RMSE
linear	0.1200419
tree	0.1072732
random forest	0.0901681

Let's practice!

SUPERVISED LEARNING IN R: REGRESSION

Random forests

SUPERVISED LEARNING IN R: REGRESSION

Nina Zumel and John Mount
Win-Vector, LCC

Random Forests

Multiple diverse decision trees averaged together

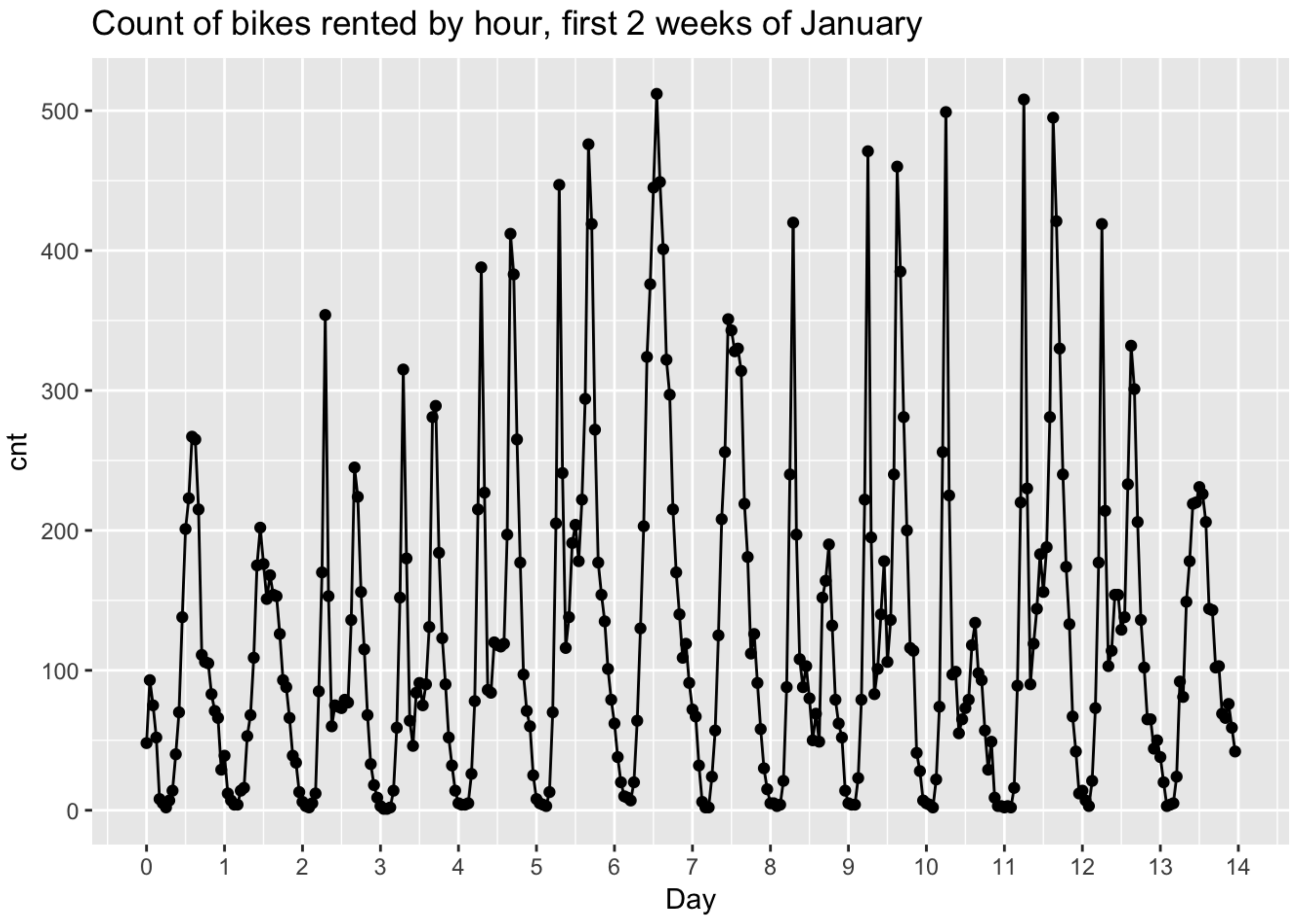
- Reduces overfit
- Increases model expressiveness
- Finer grain predictions

Building a Random Forest Model

1. Draw bootstrapped sample from training data
2. For each sample grow a tree
    - At each node, pick best variable to split on (from a random subset of all variables)
    - Continue until tree is grown
3. To score a datum, evaluate it with all the trees and average the results.

Example: Bike Rental Data

```
cnt ~ hr + holiday + workingday +
  weathersit + temp + atemp + hum + windspeed
```



Random Forests with ranger()

```
model <- ranger(fmla, bikesJan,
                num.trees = 500,
                respect.unordered.factors = "order")
```

- `formula` , `data`
- `num.trees` (default 500) - use at least 200
- `mtry` - number of variables to try at each node
  - default: square root of the total number of variables
- `respect.unordered.factors` - recommend set to "order"
  - "safe" hashing of categorical variables

Random Forests with ranger()

```
model
```

```
Ranger result
...
OOB prediction error (MSE):       3103.623
R squared (OOB):                  0.7837386
```

Random forest algorithm returns estimates of out-of-sample performance.

Predicting with a ranger() model

```
bikesFeb$pred <- predict(model, bikesFeb)$predictions
```

`predict()` inputs:

- model
- data

Predictions can be accessed in the element `predictions`.

Evaluating the model

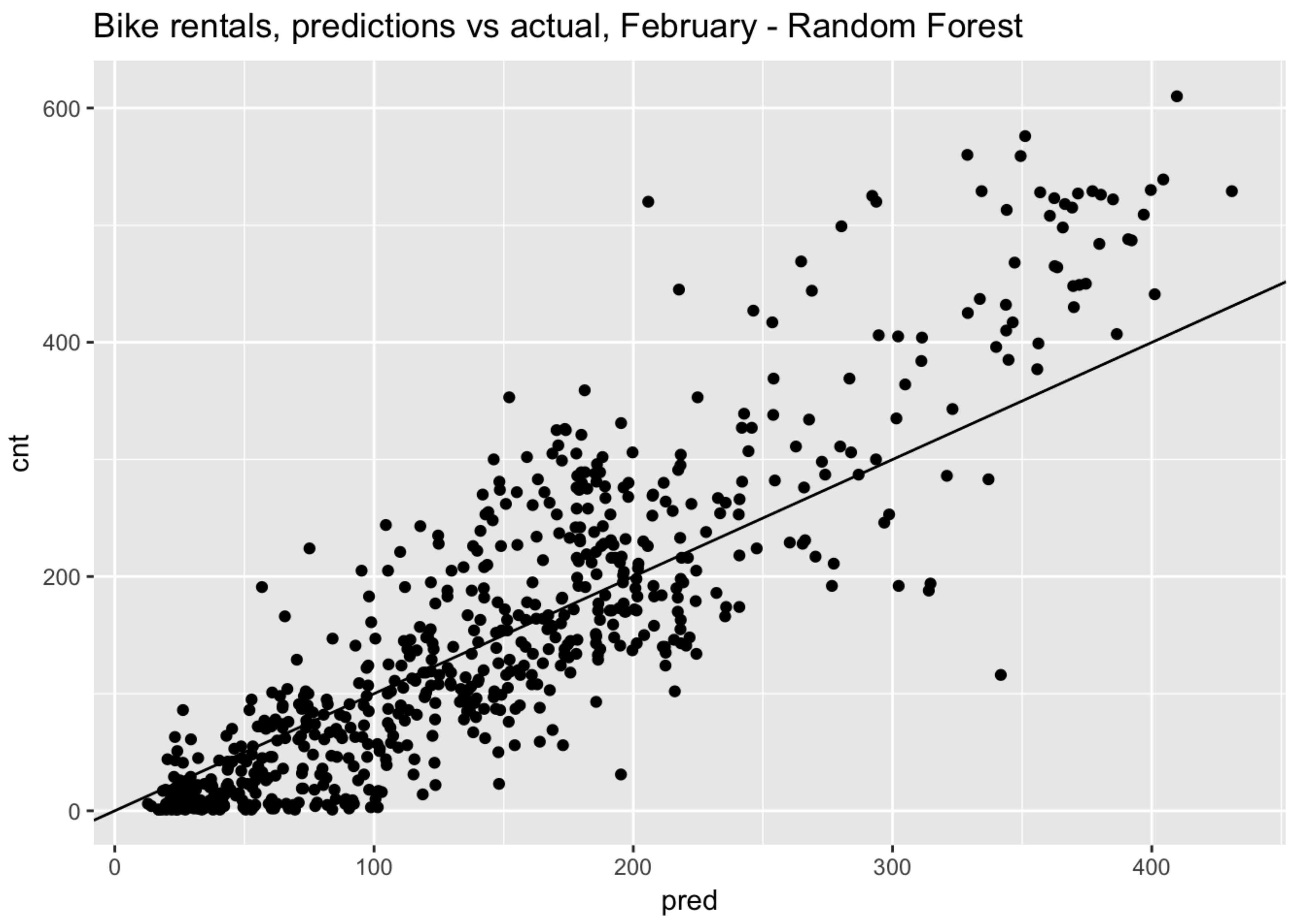
Calculate RMSE:

```
bikesFeb %>%
  mutate(residual = pred - cnt) %>%
  summarize(rmse = sqrt(mean(residual^2)))
```

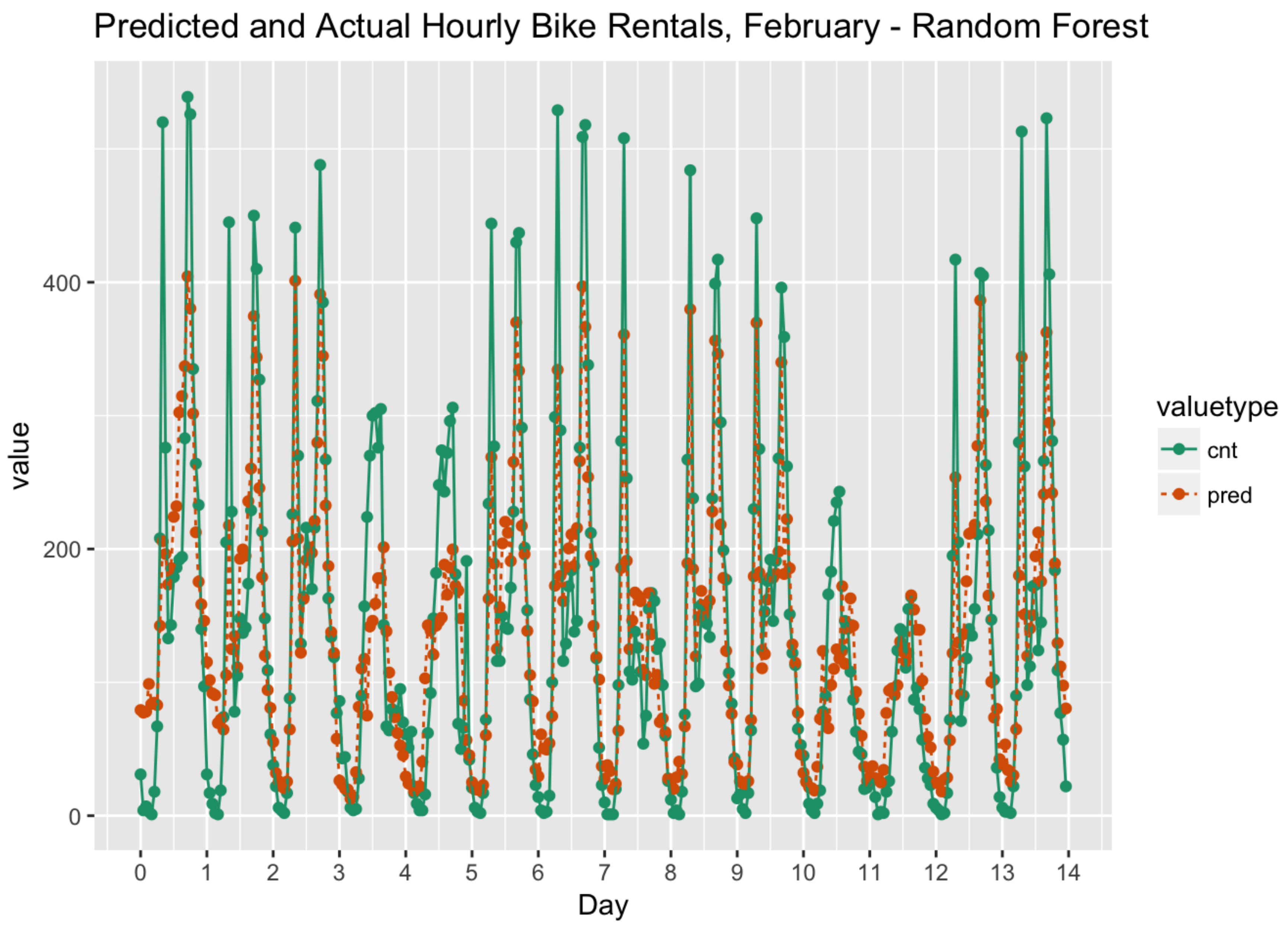
```
      rmse
1 67.15169
```

Model	RMSE
Quasipoisson	69.3
Random forests	67.15

Evaluating the model



Evaluating the model



Let's practice!

SUPERVISED LEARNING IN R: REGRESSION

One-Hot-Encoding Categorical Variables

SUPERVISED LEARNING IN R: REGRESSION

Nina Zumel and John Mount
Win-Vector, LLC

Why Convert Categoricals Manually?

- Most R functions manage the conversion for you
  - `model.matrix()`
- `xgboost()` does not
  - Must convert categorical variables to numeric representation
- Conversion to indicators: *one-hot encoding*

One-hot-encoding and data cleaning with `vtreat`

Basic idea:

- `designTreatmentsZ()` to design a *treatment plan* from the training data, then
- `prepare()` to created "clean" data
  - all numerical
  - no missing values
    - use `prepare()` with treatment plan for all future data

A Small vtreat Example

Training Data

x	u	y
one	44	0.4855671
two	24	1.3683726
three	66	2.0352837
two	22	1.6396267

Test Data

x	u	y
one	5	2.6488148
three	12	1.5012938
one	56	0.1993731
two	28	1.2778516

Create the Treatment Plan

```
vars <- c("x", "u")
treatplan <- designTreatmentsZ(dframe, varslist, verbose = FALSE)
```

Inputs to `designTreatmentsZ()`

- `dframe` : training data
- `varlist` : list of input variable names
- set verbose = FALSE to suppress progress messages

Get the New Variables

The scoreFrame describes the variable mapping and types

```
(scoreFrame <- treatplan$scoreFrame %>%
+     select(varName, origName, code))
```

```
        varName origName  code
1   x_lev_x.one        x   lev
2 x_lev_x.three        x   lev
3   x_lev_x.two        x   lev
4        x_catP        x  catP
5       u_clean        u clean
```

Get the names of the new `lev` and `clean` variables

```
(newvars <- scoreFrame %>%
+     filter(code %in% c("clean", "lev")) %>%
+     use_series(varName))
"x_lev_x.one"   "x_lev_x.three" "x_lev_x.two"   "u_clean"
```

Prepare the Training Data for Modeling

```
training.treat <- prepare(treatmentplan, dframe, varRestriction = newvars)
```

Inputs to `prepare()` :

- `treatmentplan` : treatment plan
- `dframe` : data frame
- `varRestriction` : list of variables to prepare (optional)
  - default: prepare all variables

Before and After Data Treatment

Training Data

x	u	y
one	44	0.4855671
two	24	1.3683726
three	66	2.0352837
two	22	1.6396267

Treated Training Data

x_lev_x.one	x_lev_x.three	x_lev_x.two	u_clean
1	0	0	44
0	0	1	24
0	1	0	66
0	0	1	22

Prepare the Test Data Before Model Application

```
(test.treat <- prepare(treatplan, test, varRestriction = newvars))
```

```
  x_lev_x.one x_lev_x.three x_lev_x.two u_clean
1           1             0           0       5
2           0             1           0      12
3           1             0           0      56
4           0             0           1      28
```

vtreat Treatment is Robust

Previously unseen `x` level: *four*

x	u	y
one	4	0.2331301
two	14	1.9331760
three	66	3.1251029
four	25	4.0332491

four encodes to (0, 0, 0)

```
prepare(treatplan, toomany, ...)
```

x_lev_x.one	x_lev_x.three	x_lev_x.two	u_clean
1	0	0	4
0	0	1	14
0	1	0	66
0	**0**	**0**	25

Let's practice!

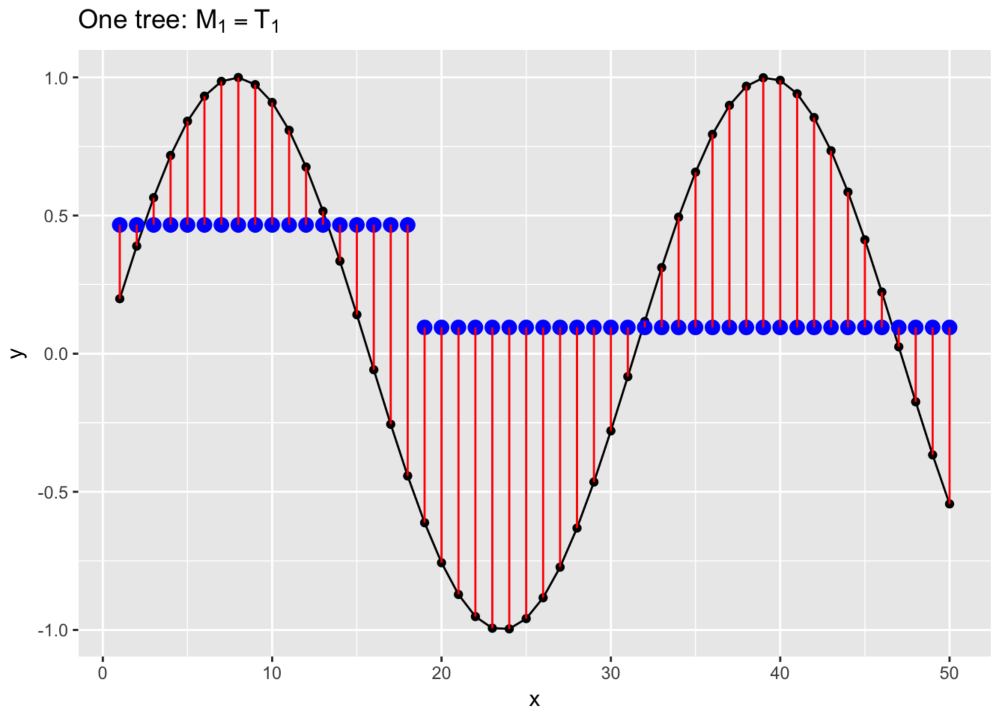
SUPERVISED LEARNING IN R: REGRESSION

Gradient boosting machines

SUPERVISED LEARNING IN R: REGRESSION

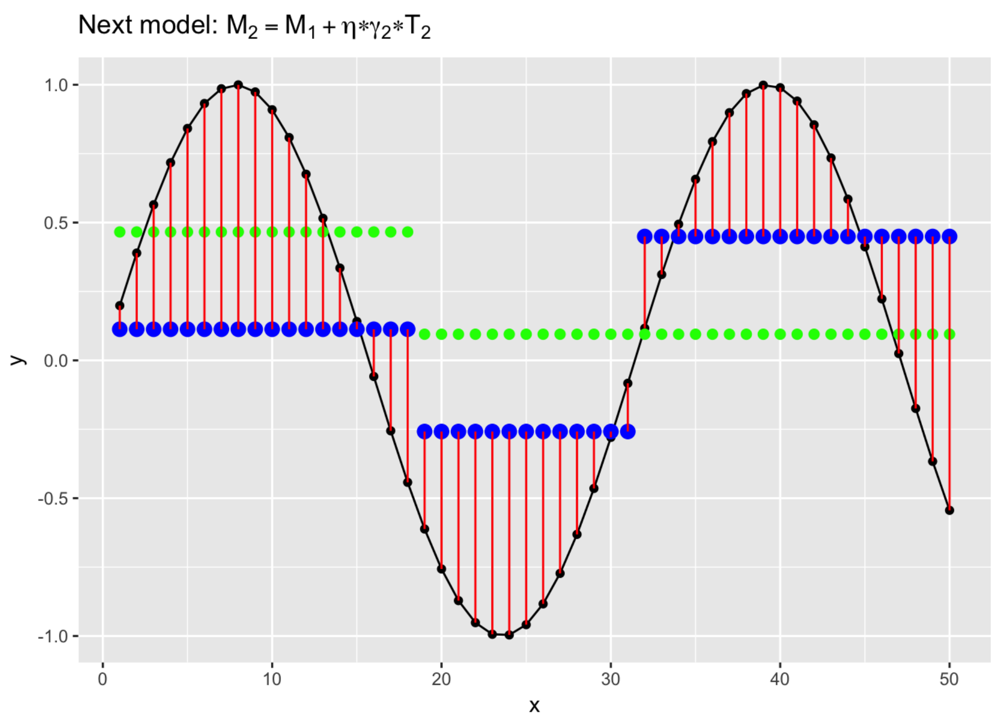
Nina Zumel and John Mount
Win-Vector, LLC

How Gradient Boosting Works



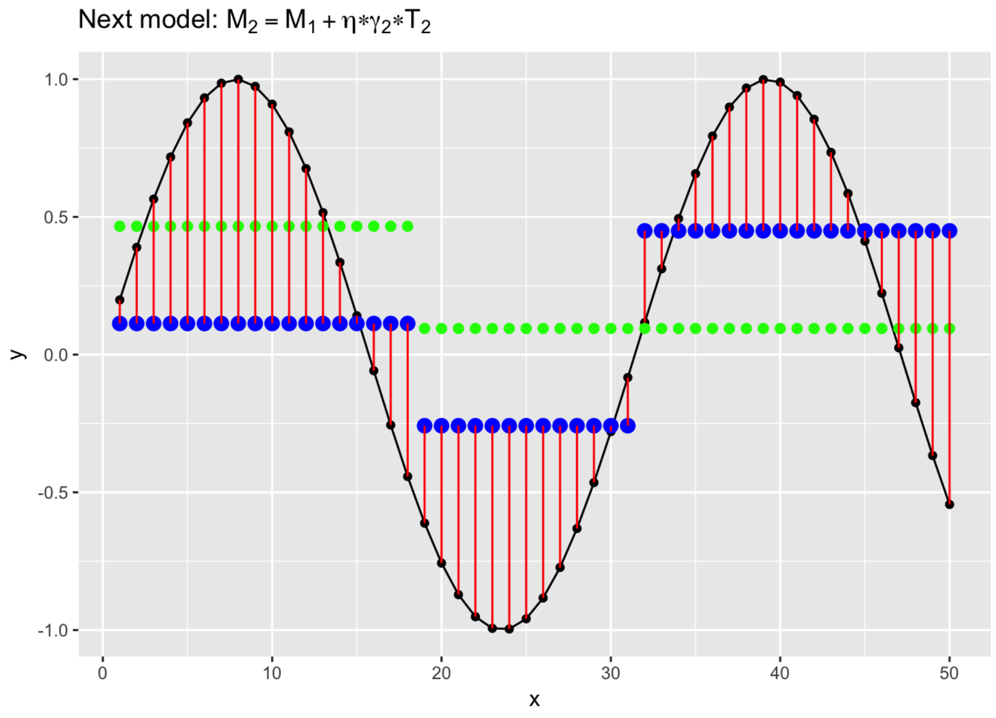
1. Fit a shallow tree T_1 to the data: $M_1 = T_1$

How Gradient Boosting Works



1. Fit a shallow tree T_1 to the data: $M_1 = T_1$
2. Fit a tree T_2 to the residuals. Find γ such that $M_2 = M_1 + \gamma T_2$ is the best fit to data

How Gradient Boosting Works



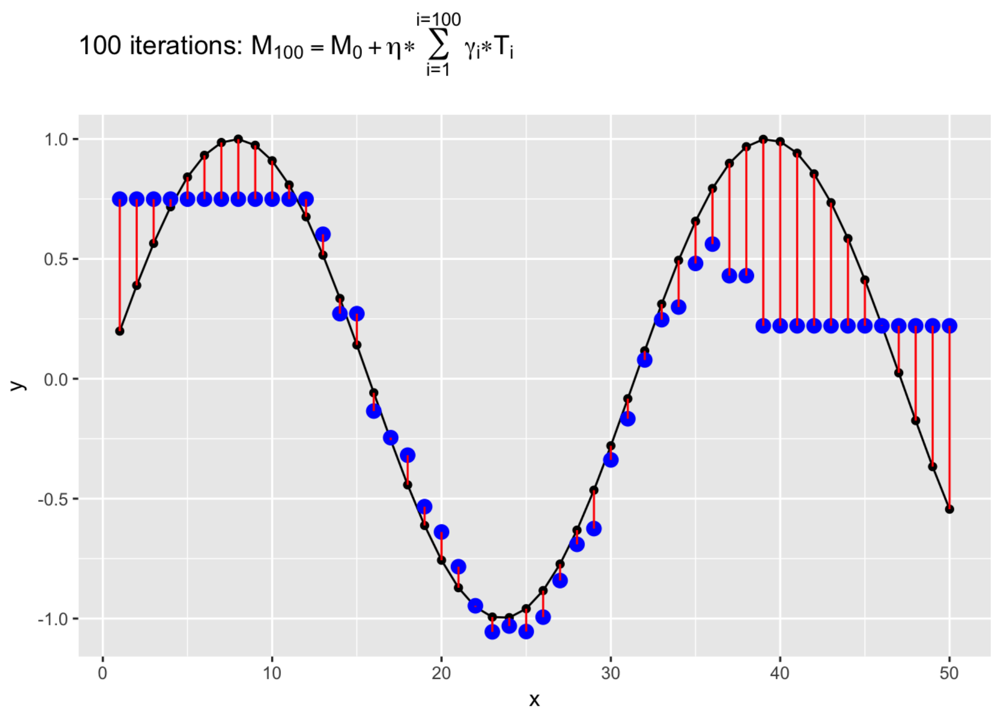
Regularization: learning rate

$\eta \in (0, 1)$

$$ M_2 = M_1 %20 \eta
\gamma T_2 $$

- Larger η: faster learning
- Smaller η: less risk of overfit

How Gradient Boosting Works

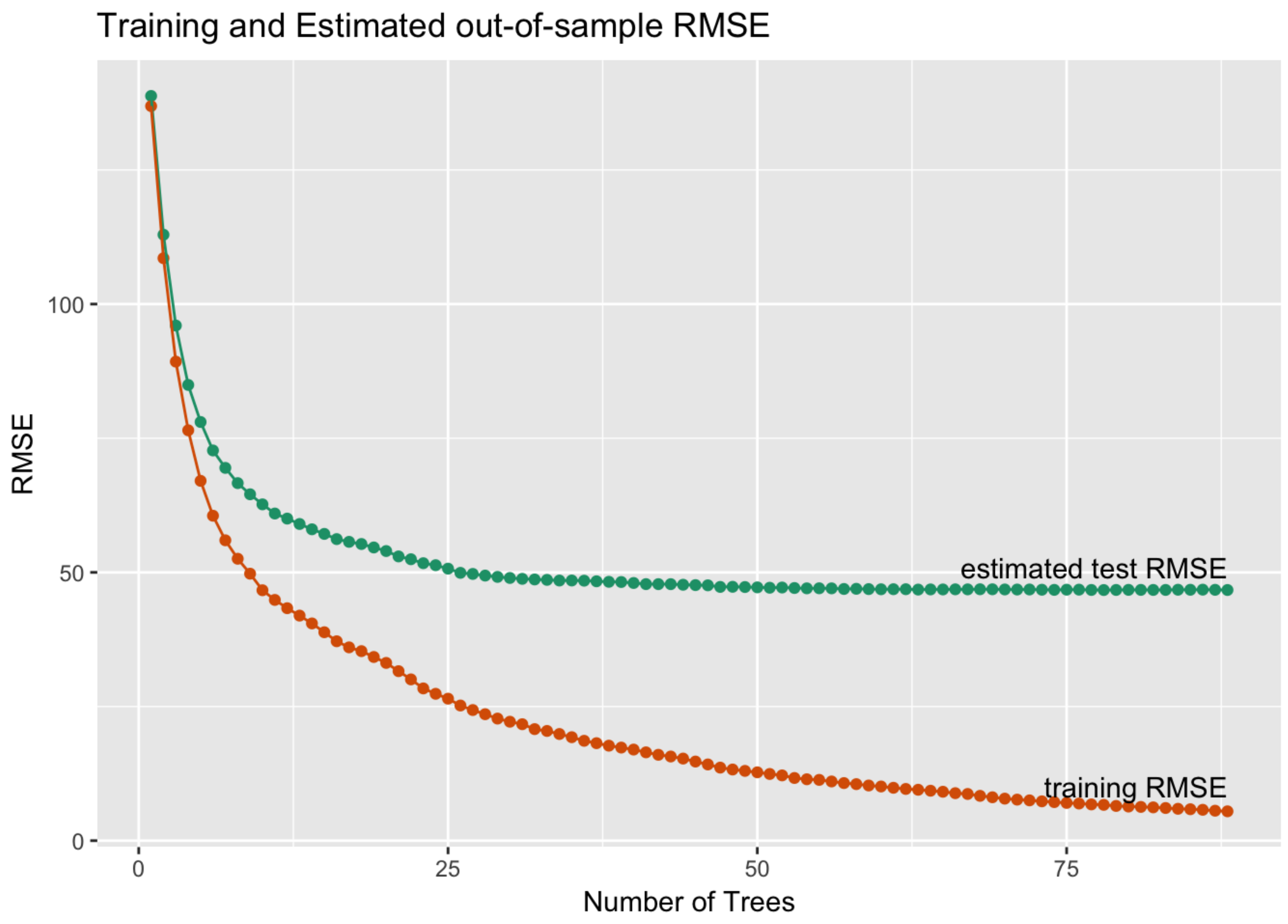


1. Fit a shallow tree T_1 to the data
   - $M_1 = T_1$
2. Fit a tree T_2 to the residuals.
   - $M_2 = M_1 + \eta\gamma_2 T_2$
3. Repeat (2) until stopping condition met

Final Model:

$$M = M_1 + \eta \sum \gamma_i T_i$$

Cross-validation to Guard Against Overfit



Training error keeps decreasing, but test error doesn't

Best Practice (with xgboost())

1. Run `xgb.cv()` with a large number of rounds (trees).

Best Practice (with xgboost())

1. Run `xgb.cv()` with a large number of rounds (trees).
2. `xgb.cv()$evaluation_log` : records estimated RMSE for each round.
   - Find the number of trees that minimizes estimated RMSE: n_{best}

Best Practice (with xgboost())

1. Run `xgb.cv()` with a large number of rounds (trees).
2. `xgb.cv()$evaluation_log` : records estimated RMSE for each round.
   - Find the number of trees that minimizes estimated RMSE: n_{best}
3. Run `xgboost()` , setting `nrounds` = n_{best}

Example: Bike Rental Model

First, prepare the data

```
treatplan <- designTreatmentsZ(bikesJan, vars)
newvars <- treatplan$scoreFrame %>%
+     filter(code %in% c("clean", "lev")) %>%
+     use_series(varName)

bikesJan.treat <- prepare(treatplan, bikesJan, varRestriction = newvars)
```

For `xgboost()` :

- Input data: `as.matrix(bikesJan.treat)`
- Outcome: `bikesJan$cnt`

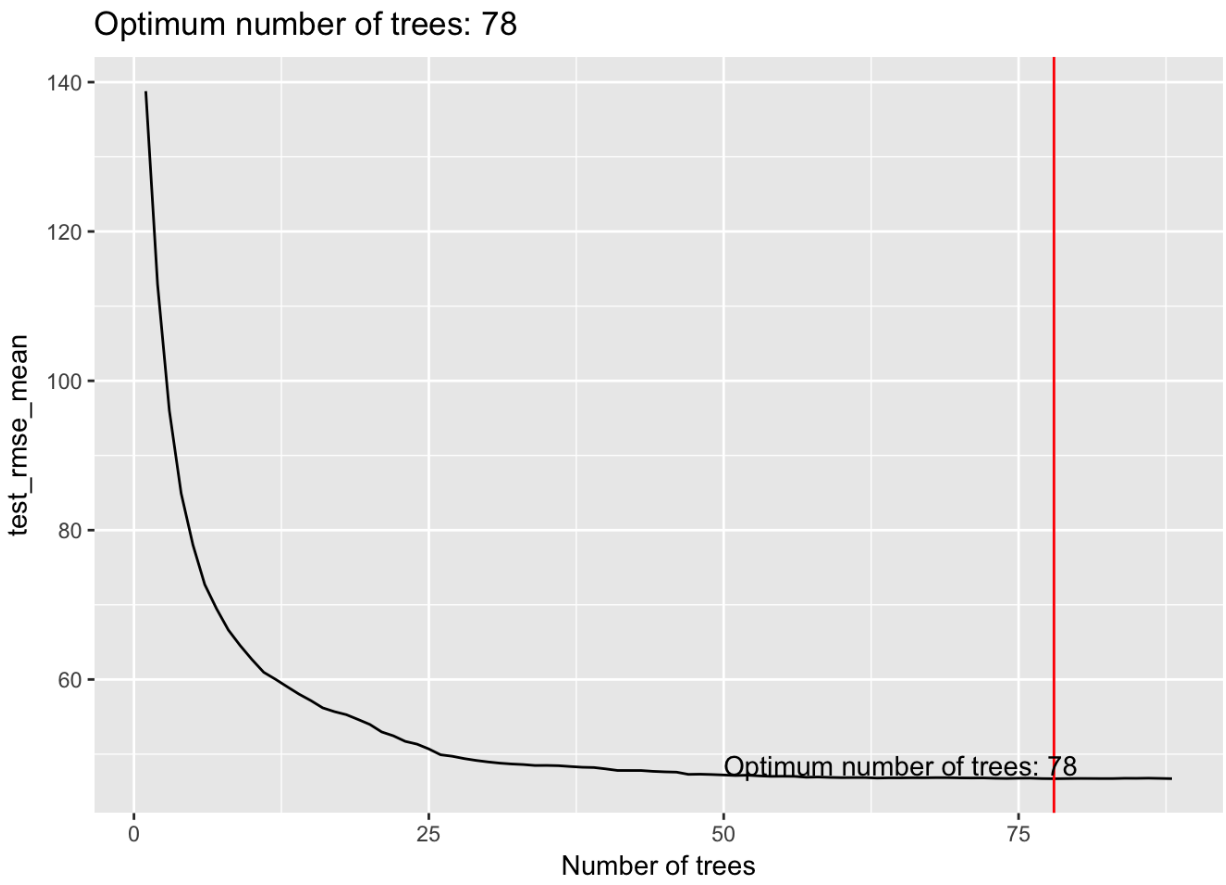
Training a model with xgboost() / xgb.cv()

```
cv <- xgb.cv(data = as.matrix(bikesJan.treat),
+              label = bikesJan$cnt,
+              objective = "reg:linear",
+              nrounds = 100, nfold = 5, eta = 0.3, depth = 6)
```

Key inputs to `xgb.cv()` and `xgboost()`

- `data` : input data as matrix ; `label` : outcome
- `objective` : for regression - "reg:linear"
- `nrounds` : maximum number of trees to fit
- `eta` : learning rate
- `depth` : maximum depth of individual trees
- `nfold` (`xgb.cv()` only): number of folds for cross validation

Find the Right Number of Trees




```
elog <- as.data.frame(cv$evaluation_log)
(nrounds <- which.min(elog$test_rmse_mean))
```

```
78
```

Run xgboost() for final model

```
nrounds <- 78

model <- xgboost(data = as.matrix(bikesJan.treat),
                 label = bikesJan$cnt,
                 nrounds = nrounds,
                 objective = "reg:linear",
                 eta = 0.3,
                 depth = 6)
```

Predict with an xgboost() model

Prepare February data, and predict

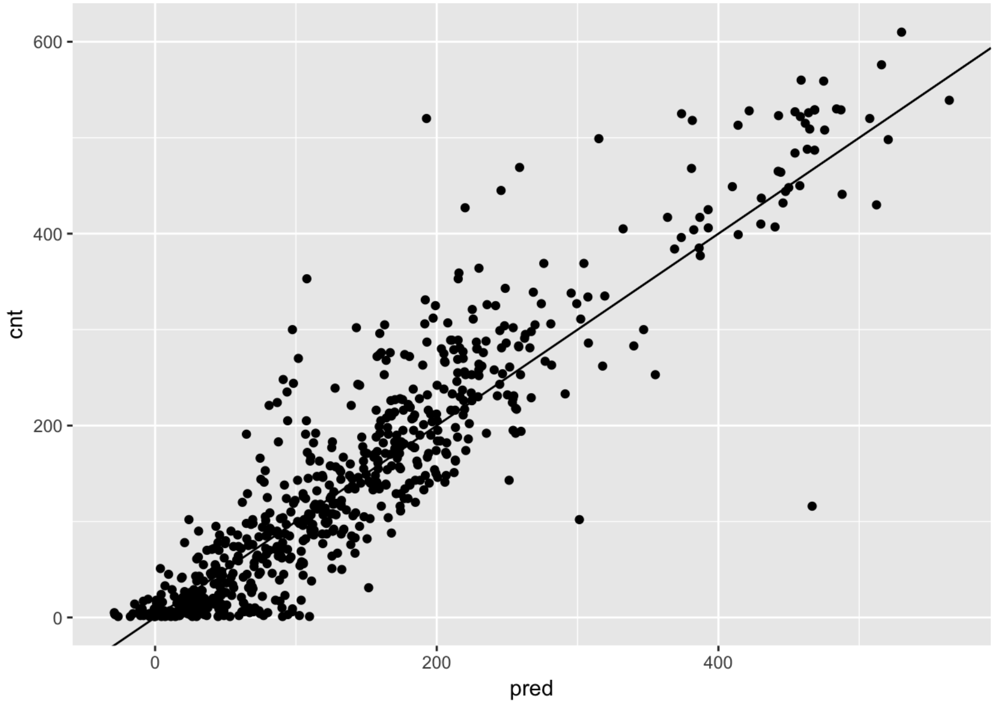
```
bikesFeb.treat <- prepare(treatplan, bikesFeb, varRestriction = newvars)

bikesFeb$pred <- predict(model, as.matrix(bikesFeb.treat))
```

Model performances on Febrary Data

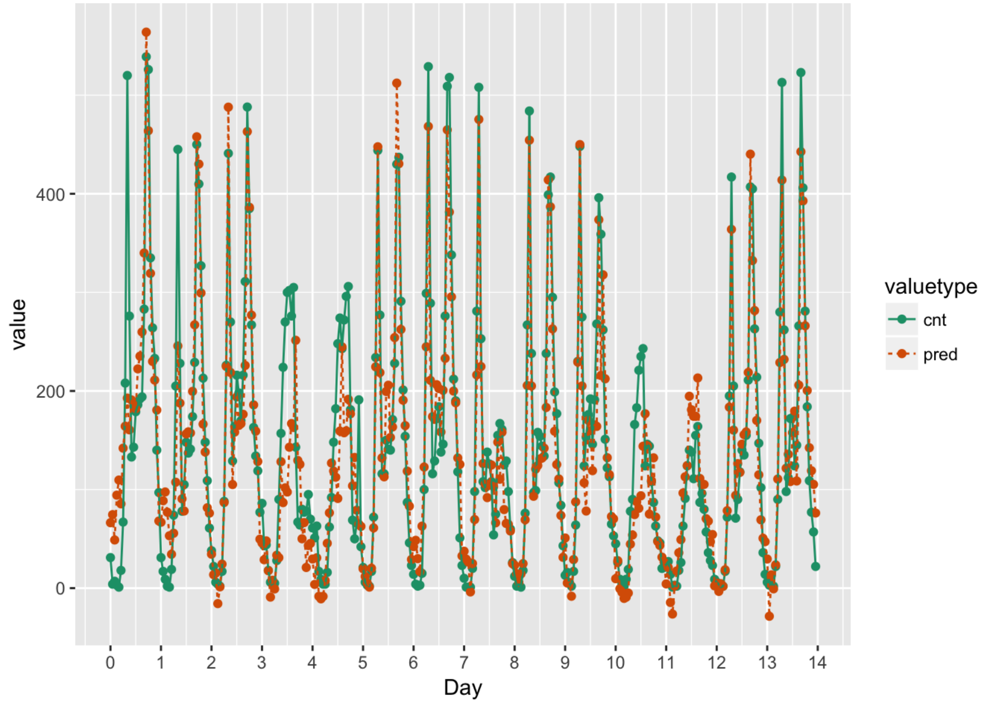
Model	RMSE
Quasipoisson	69.3
Random forests	67.15
Gradient Boosting	**54.0**

Visualize the Results

Predictions vs. Actual Bike Rentals, February



Predictions and Hourly Bike Rentals, February



Let's practice!

SUPERVISED LEARNING IN R: REGRESSION