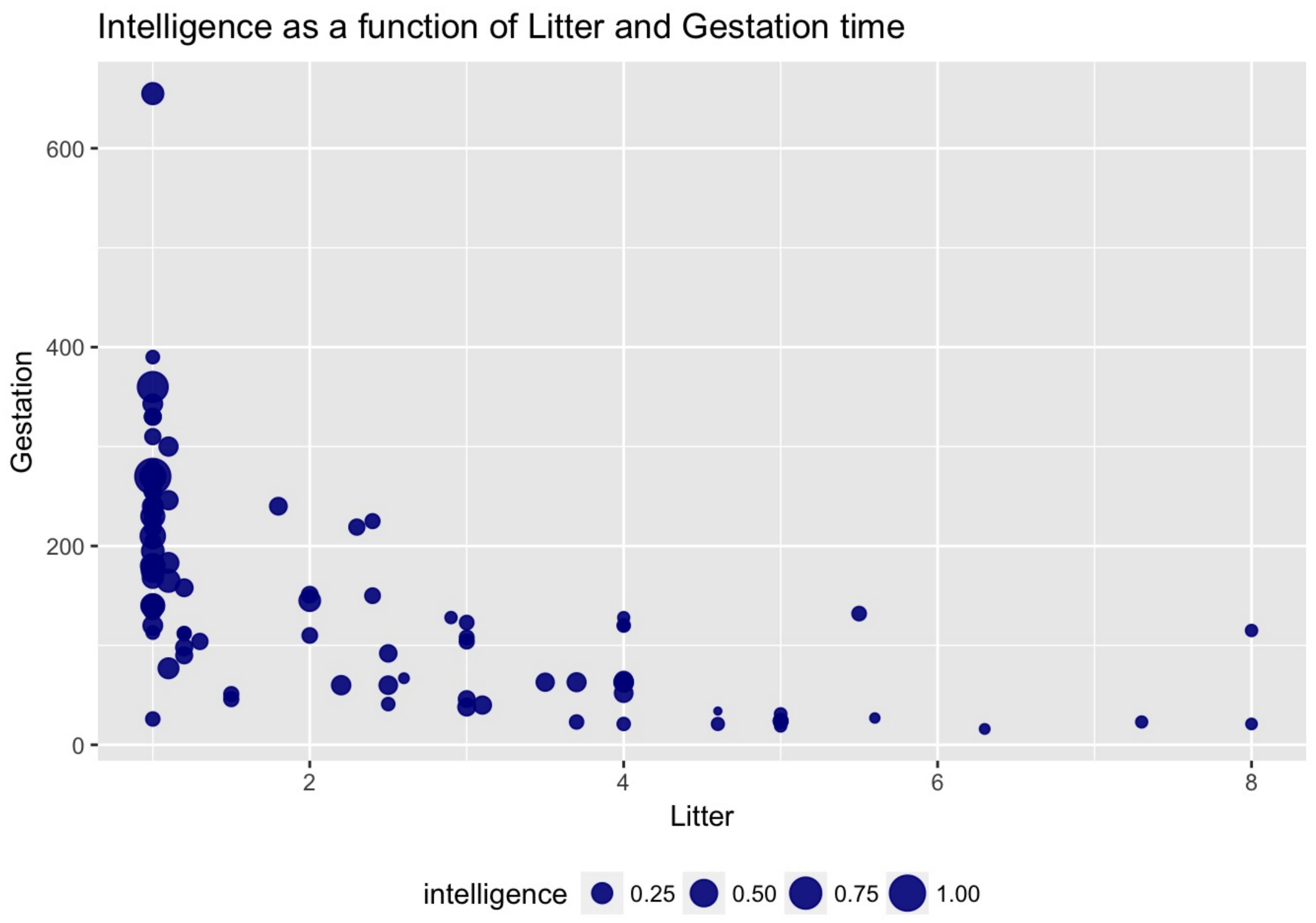
SUPERVISED LEARNING IN R: REGRESSION

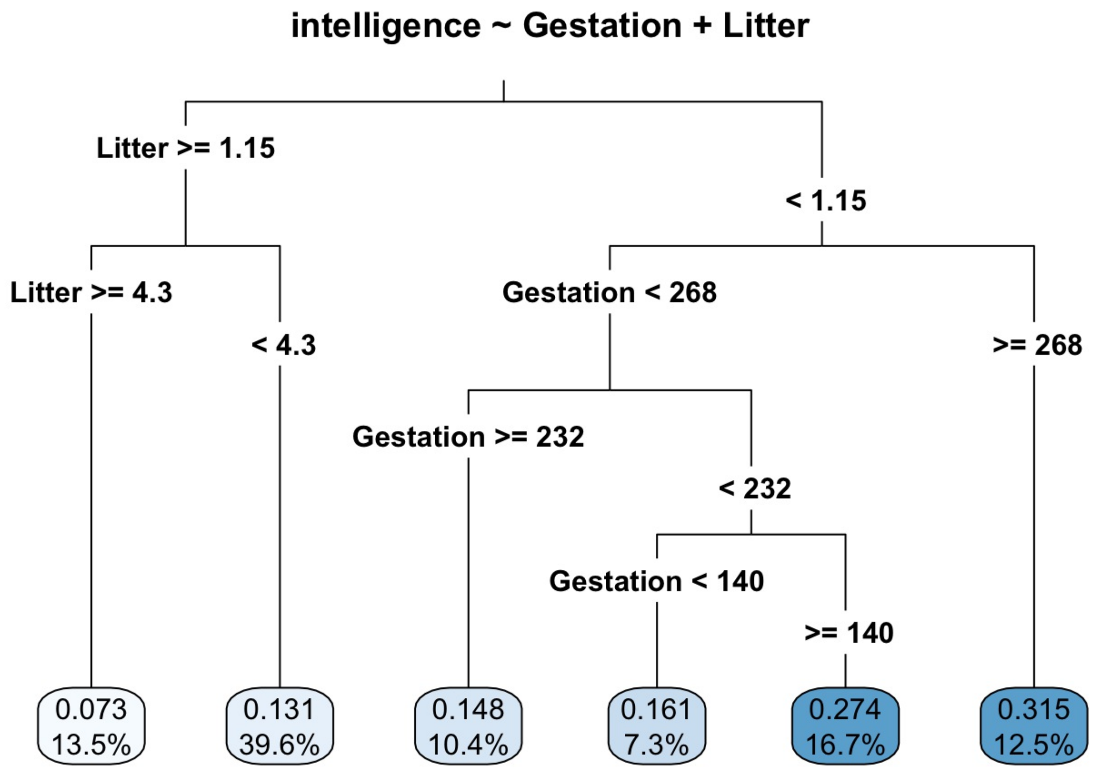
The intuition behind tree-based methods

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*

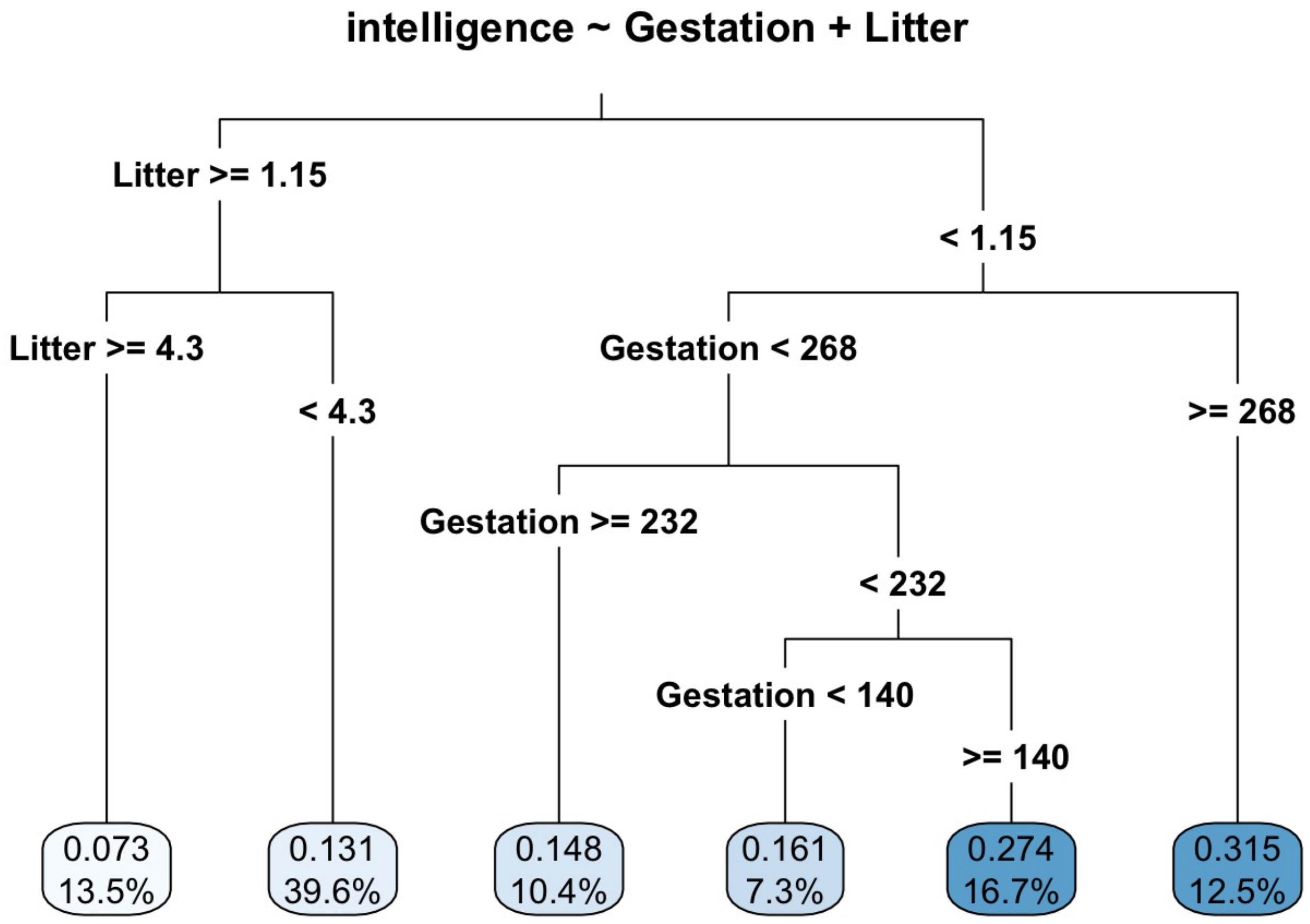
Non-linear concepts

- intervals
- non-monotonic relationships

non-additive interactions

- AND: similar to multiplication

Decision Trees



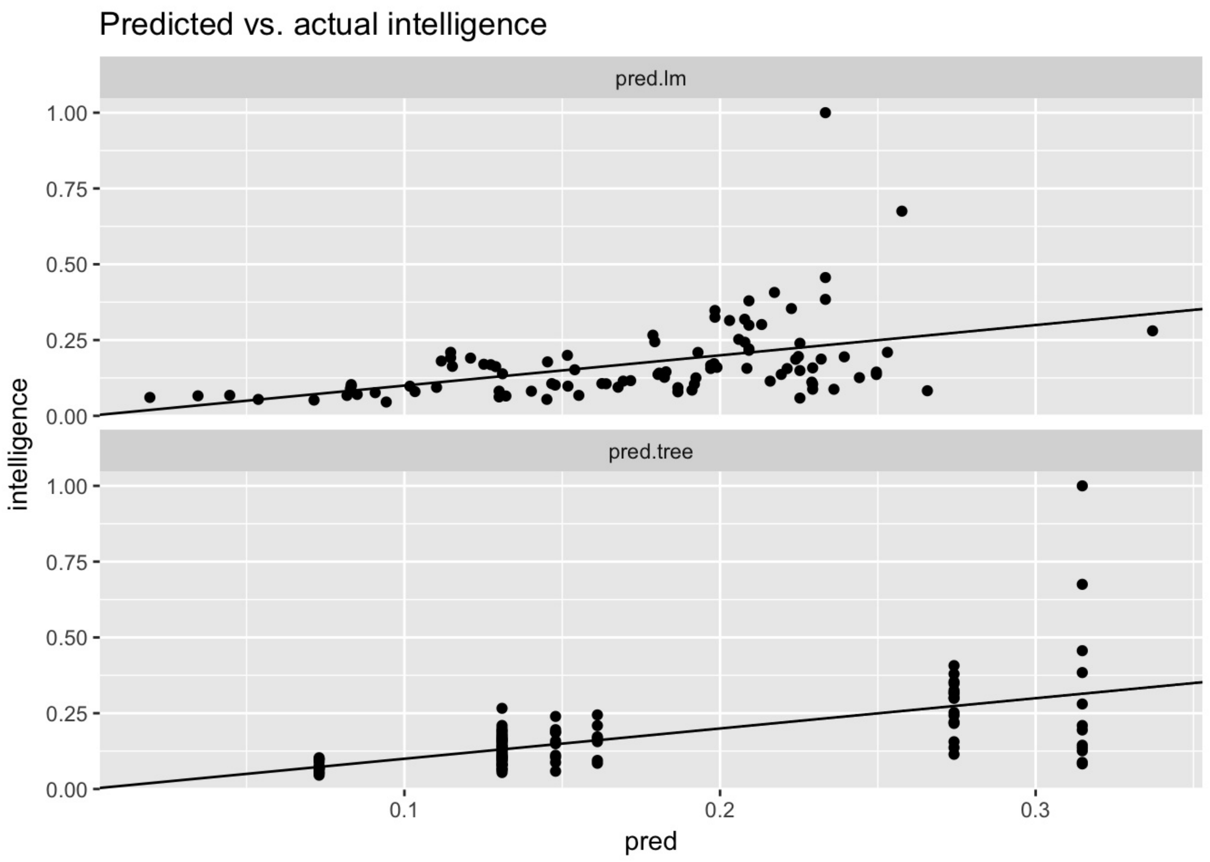
- IF Litter < 1.15 AND Gestation $\geq$ 268 $\rightarrow$ intelligence = 0.315
- IF Litter IN [1.15, 4.3) $\rightarrow$ intelligence = 0.131

Decision Trees

Pro: Trees Have an *Expressive Concept Space*

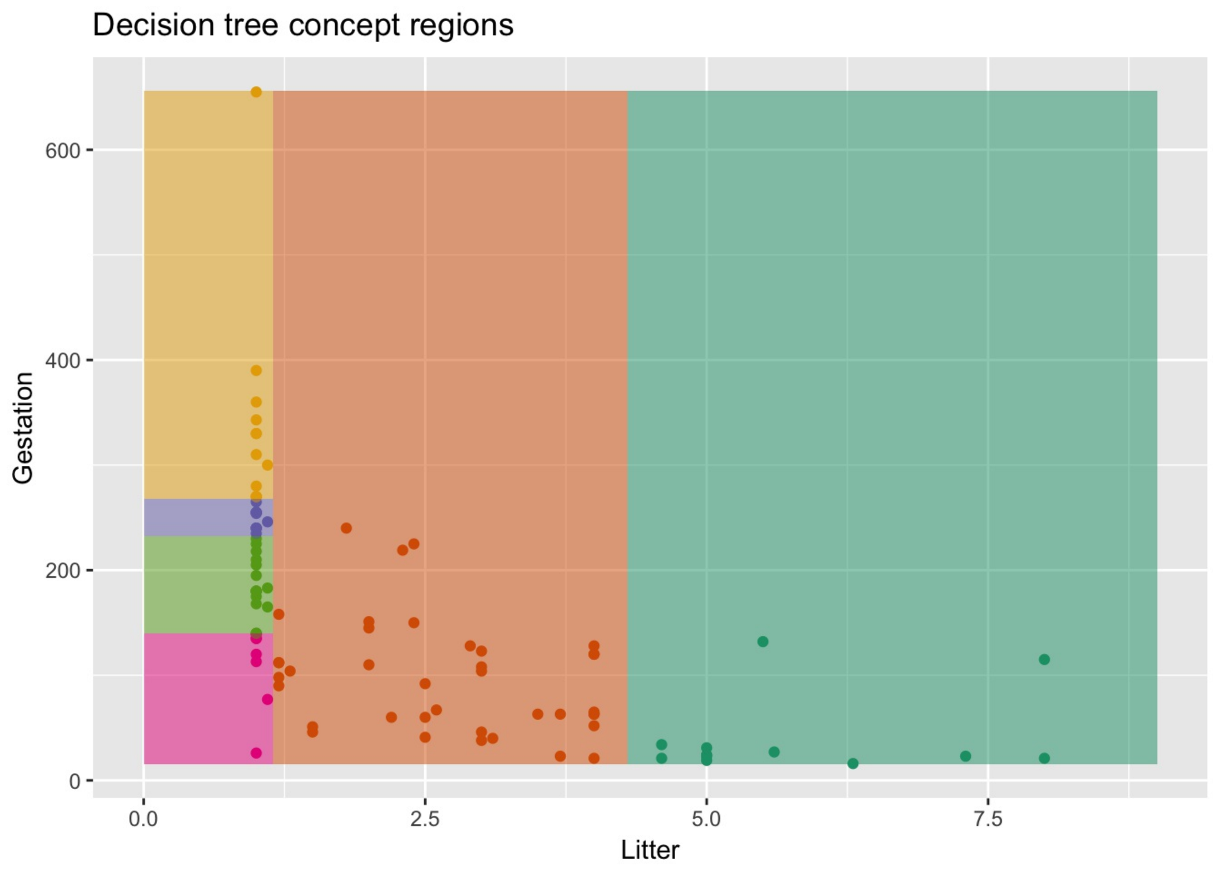
Model	RMSE
linear	0.1200419
tree	0.1072732

Con: *Coarse-Grained Predictions*



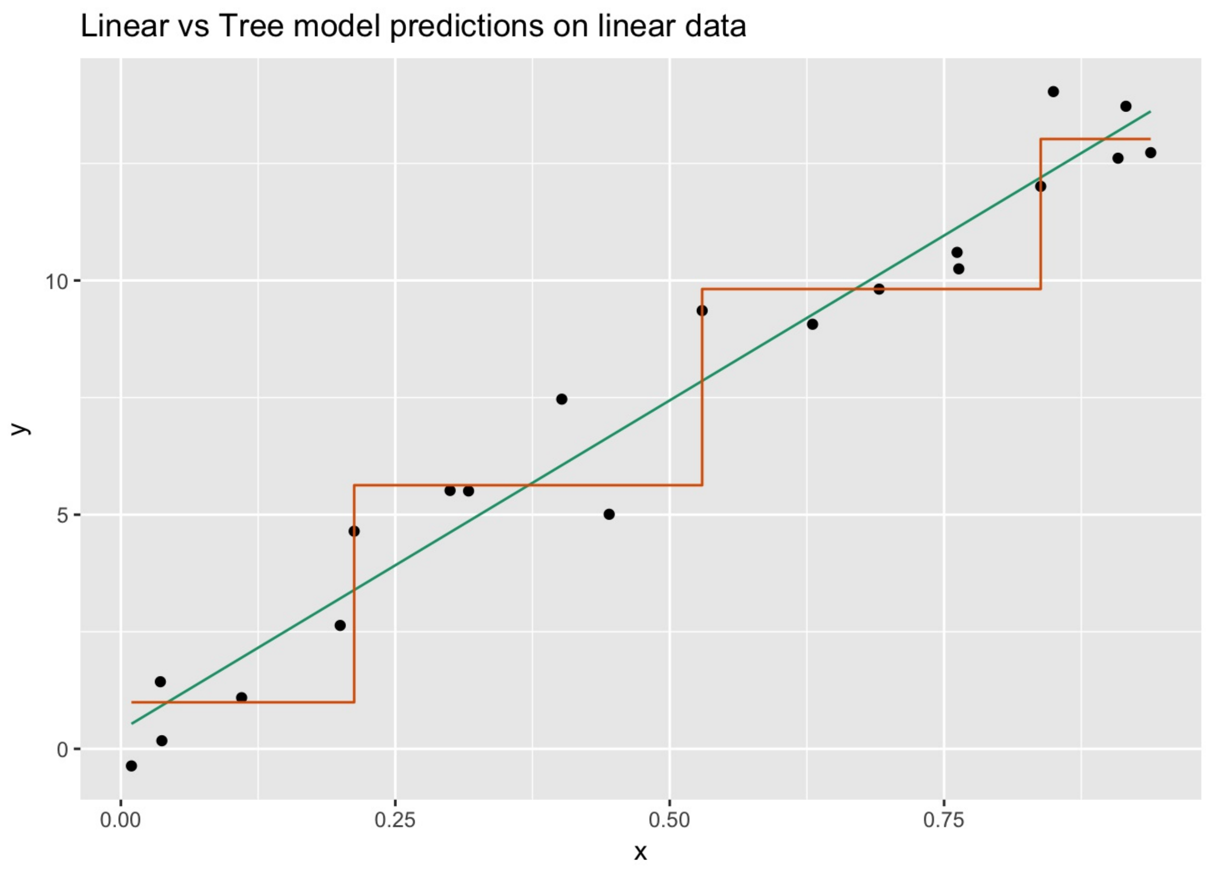
It's Hard for Trees to Express Linear Relationships

Trees Predict Axis-Aligned Regions



Each color is a different predicted value

It's Hard to Express Lines with Steps



Other Issues with Trees

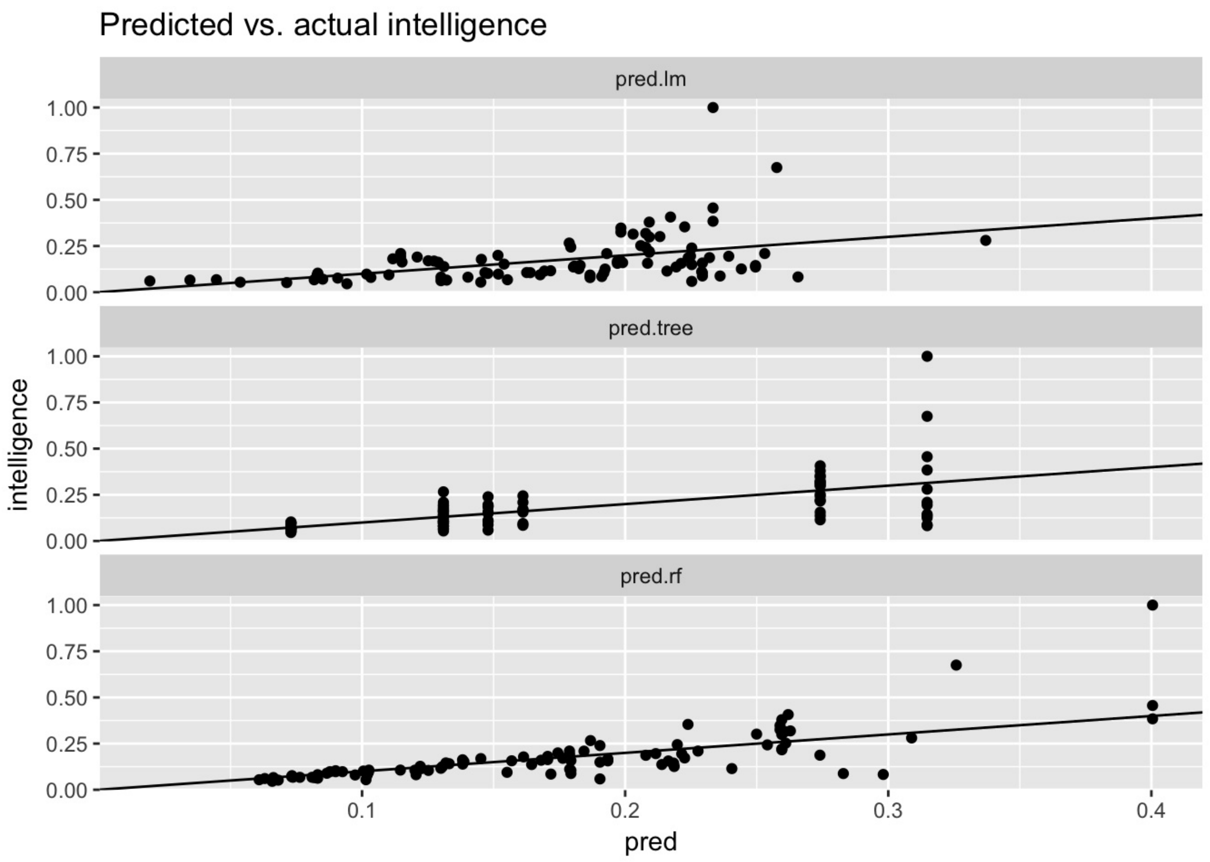
- Tree with too many splits (deep tree):
  - Too complex - danger of overfit
- Tree with too few splits (shallow tree):
  - Predictions too coarse-grained

Ensembles of Trees

Ensemble Model Fits Animal Intelligence Data Better than Single Tree

Model	RMSE
linear	0.1200419
tree	0.1072732
random forest	0.0901681

Ensembles Give Finer-grained Predictions than Single Trees



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Let's practice!

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Random forests

Nina Zumel and John Mount
Win-Vector, LCC

Random Forests

Multiple diverse decision trees averaged together

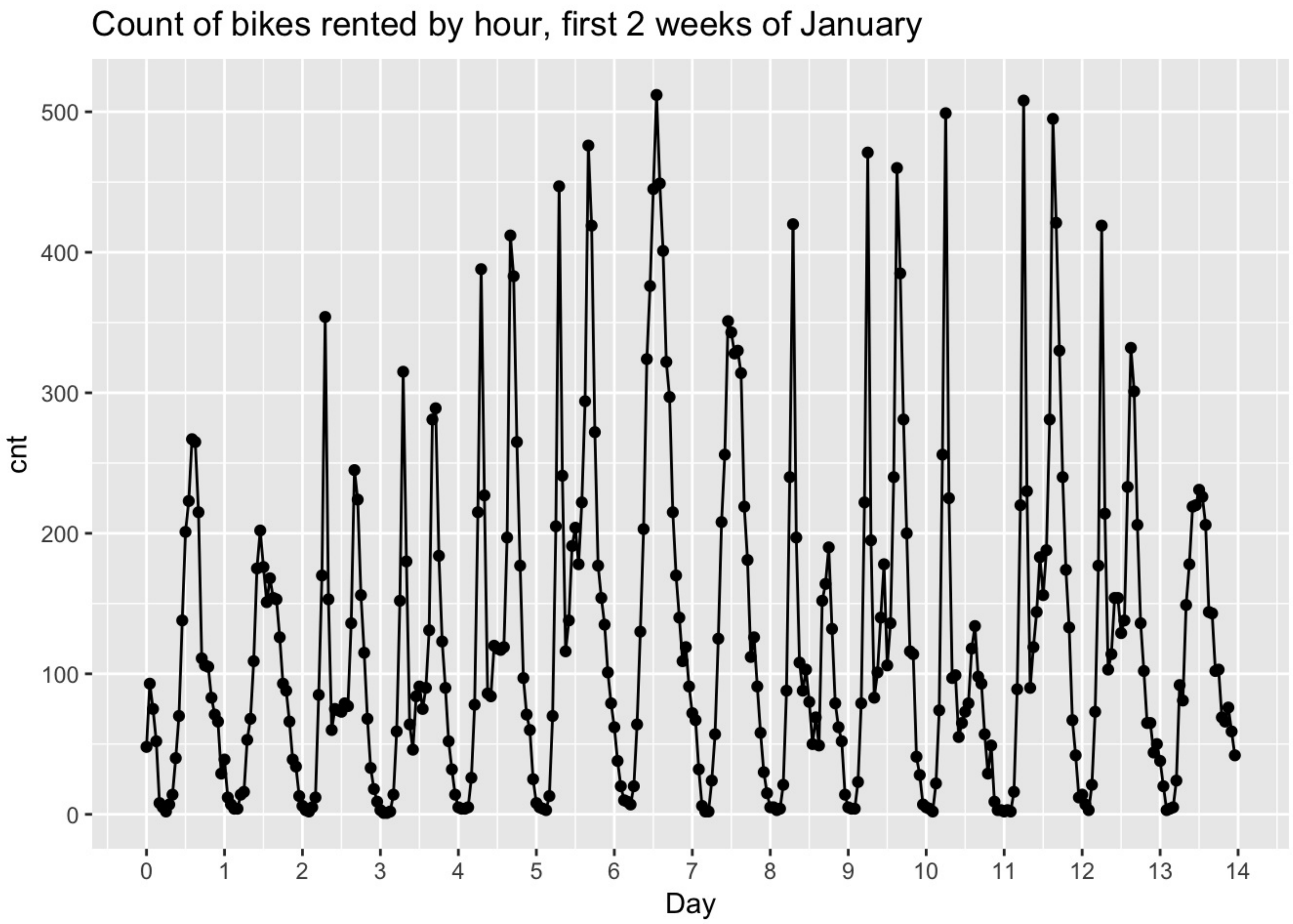
- Reduces overfit
- Increases model expressiveness
- Finer grain predictions

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

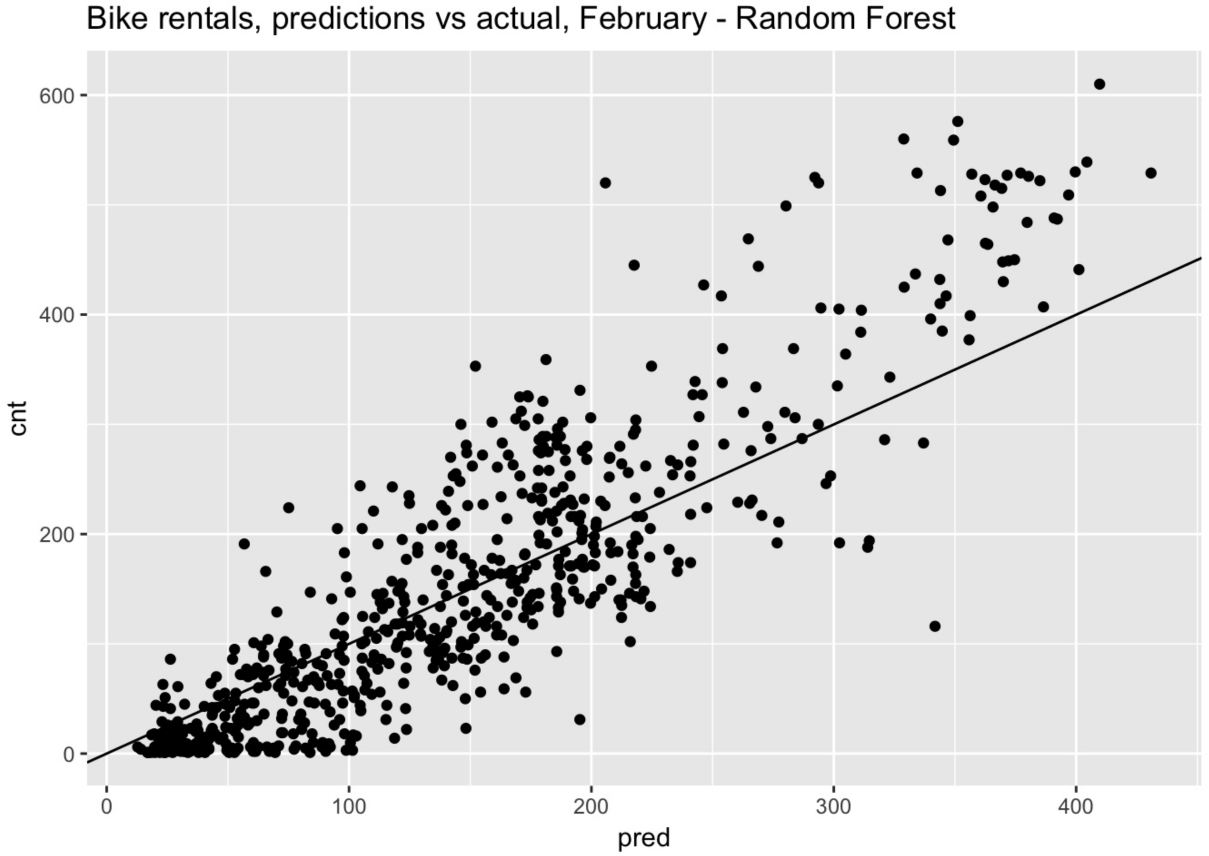
Calculate RMSE:

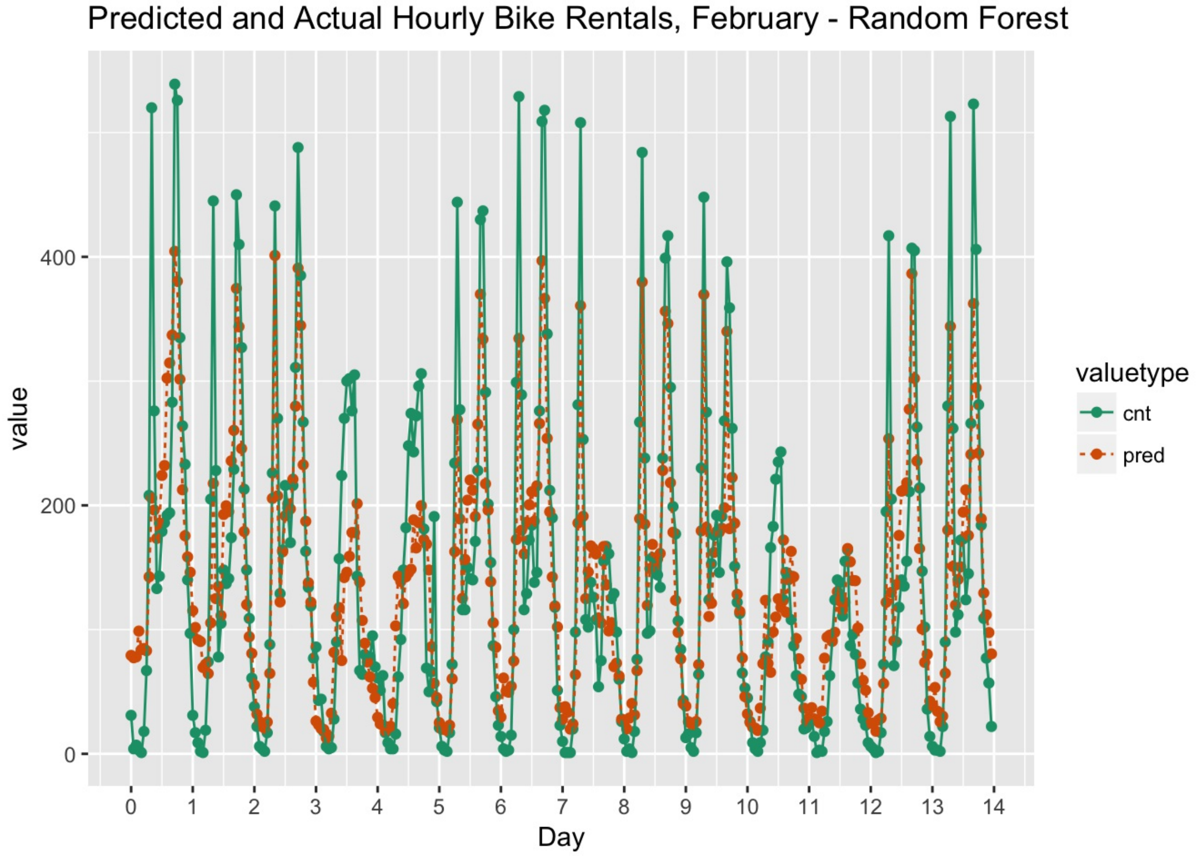
```
> bikesFeb %>%
+     mutate(residual = pred - cnt) %>%
+     summarize(rmse = sqrt(mean(residual^2)))

##       rmse
## 1 67.15169
```

Model	RMSE
Quasipoisson	69.3
Random forests	67.15

Evaluating the model





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One-Hot-Encoding Categorical Variables

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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))
[1] "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

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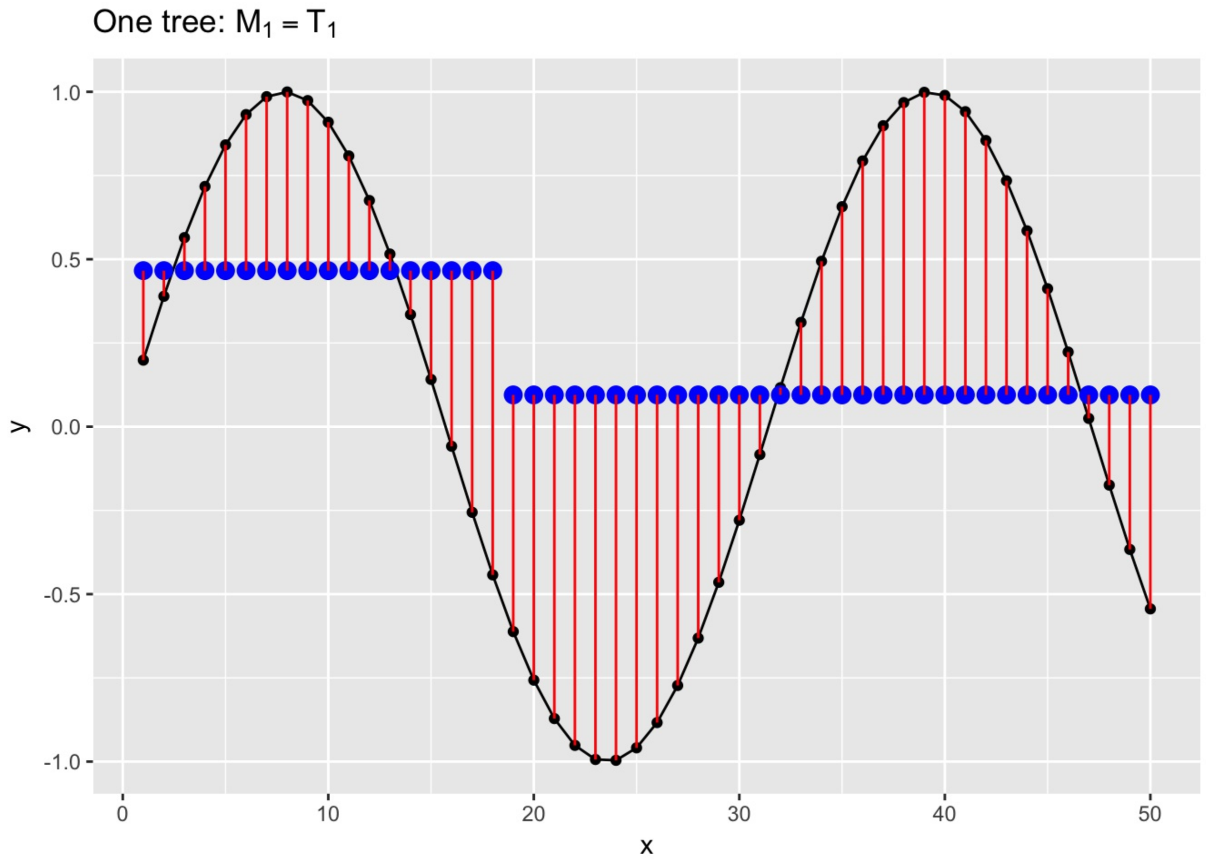
Gradient boosting machines

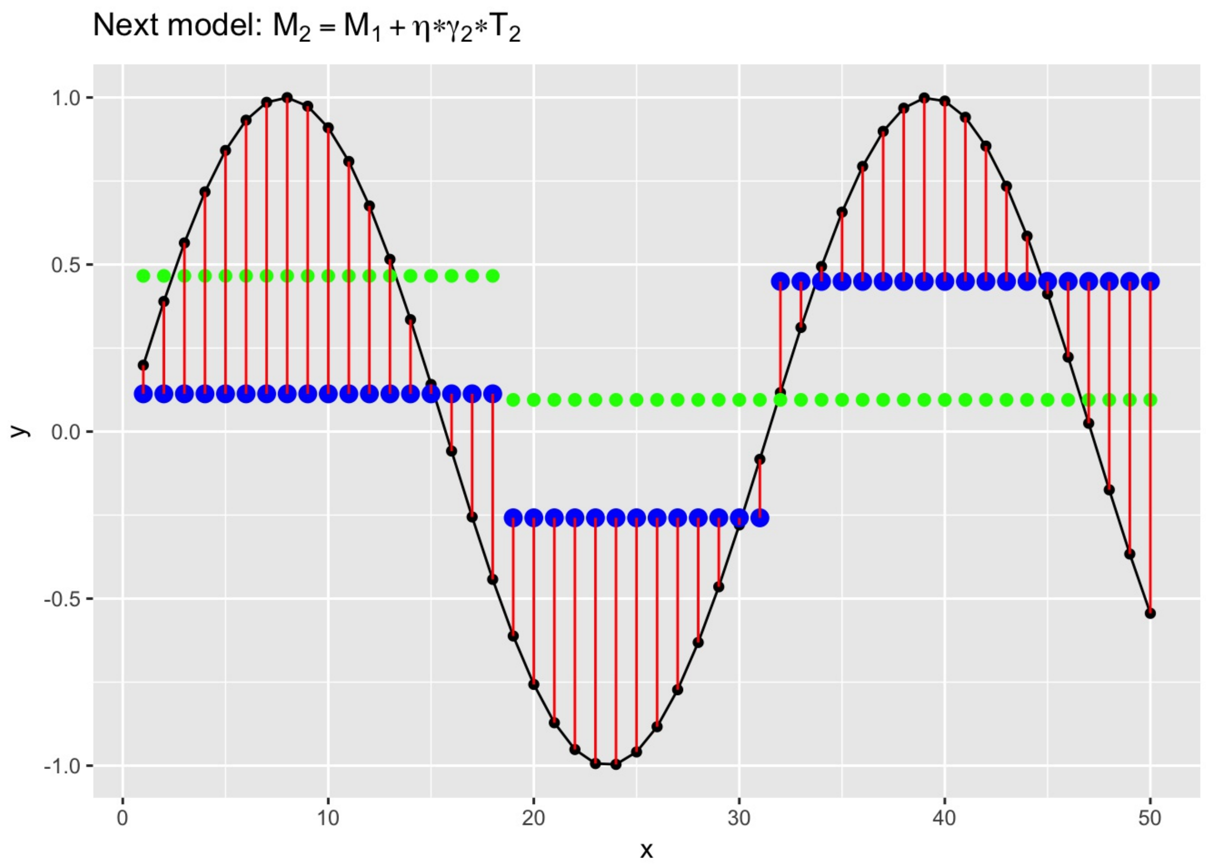
Nina Zumel and John Mount
Win-Vector, LLC

How Gradient Boosting Works



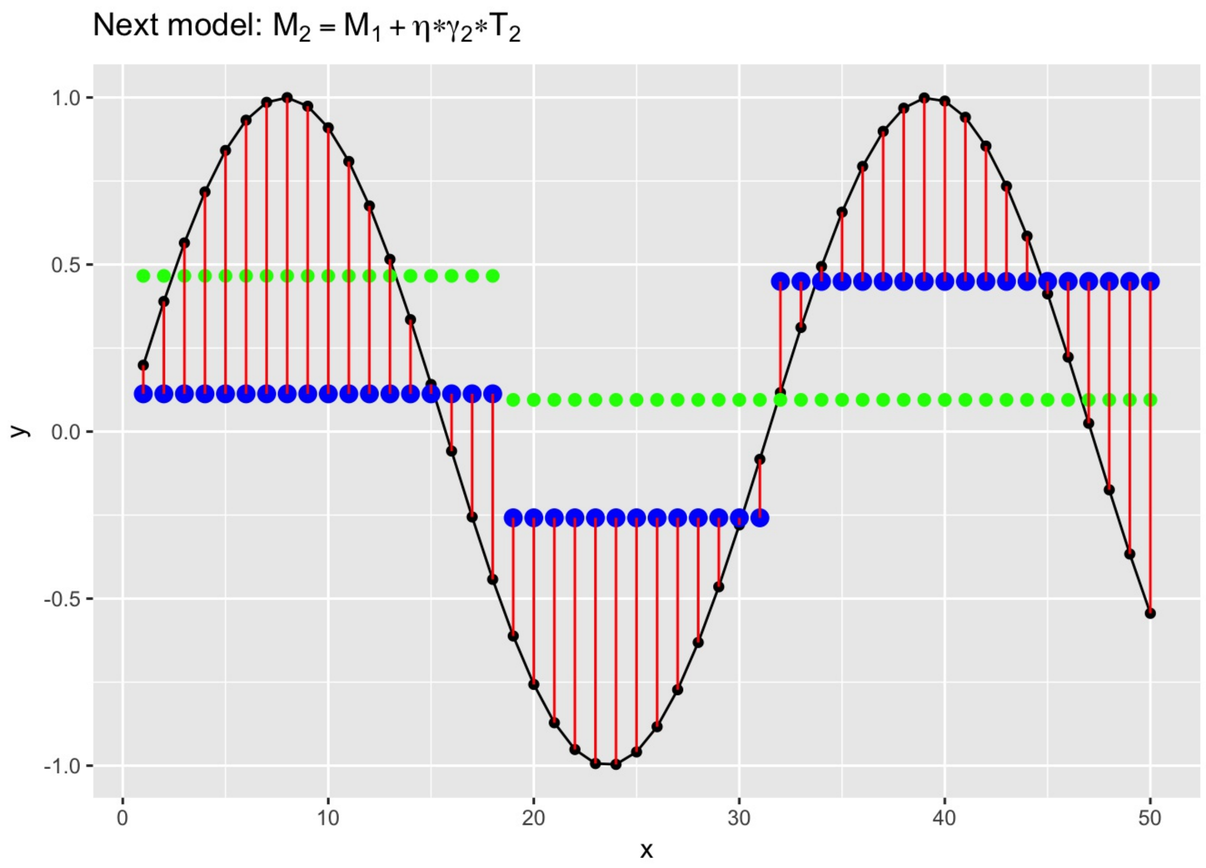
1. Fit a shallow tree T_1 to the data: $M_1 = T_1$

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

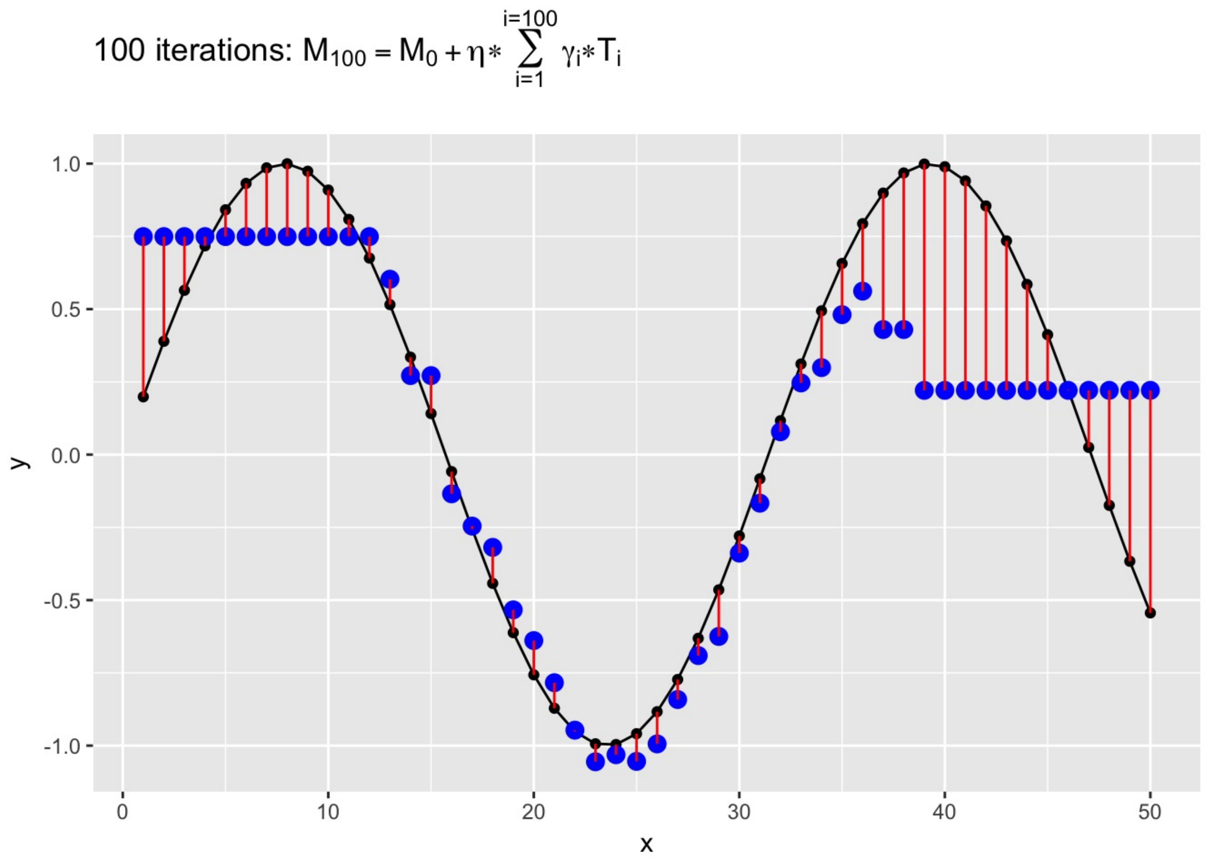


Regularization: learning rate
$\eta \in (0, 1)$

$$M_2 = M_1 + \eta\gamma T_2$$

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

How Gradient Boosting Works

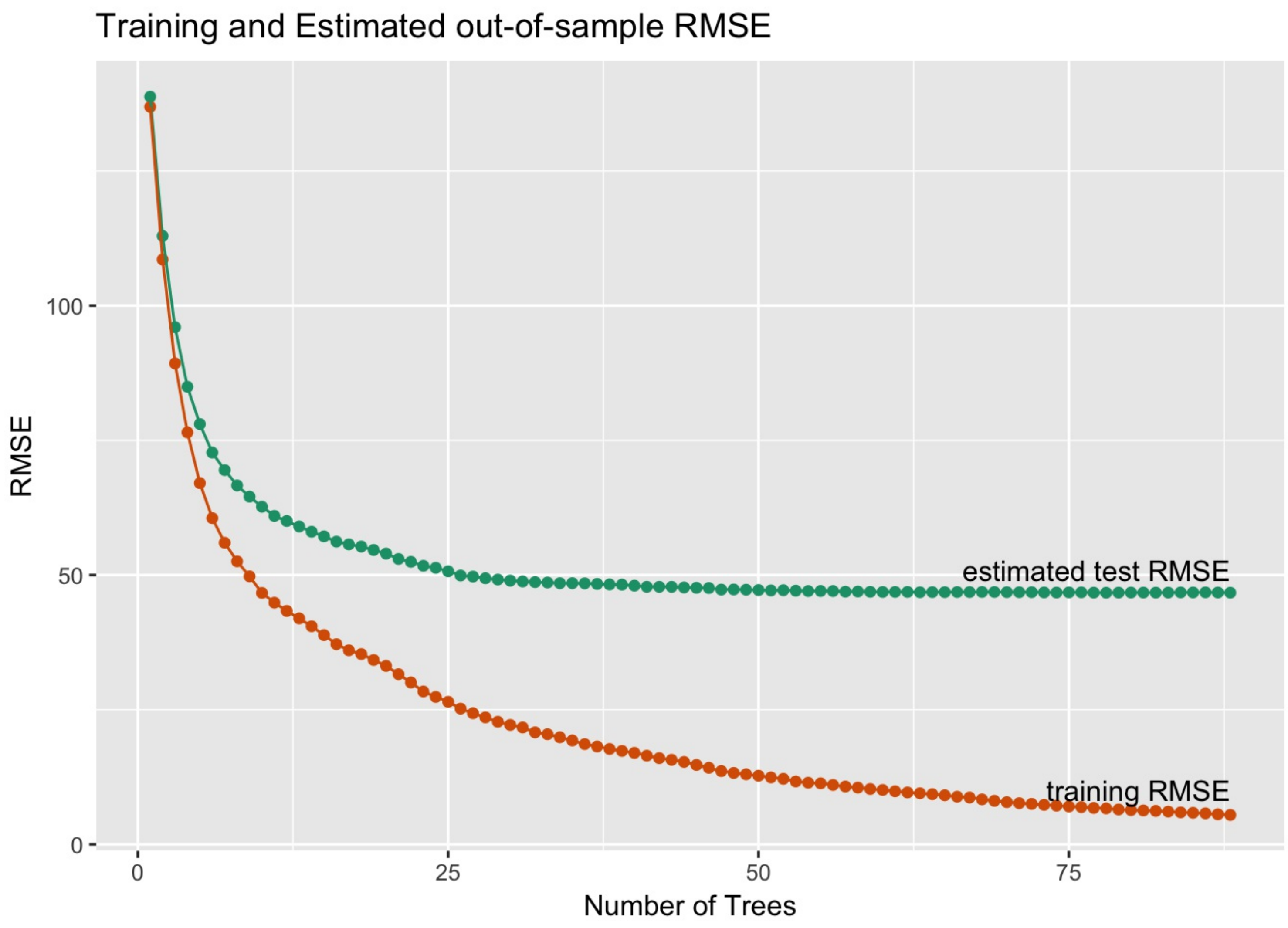


1. Fit a shallow tree T_1 to the data
   - $M_1 = T_1$
2. Fit a tree T_2 to the residuals.
   - $M_2 = M_1 + \eta\gamma_2 T_2$
3. Repeat (2) until stopping condition met

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())

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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

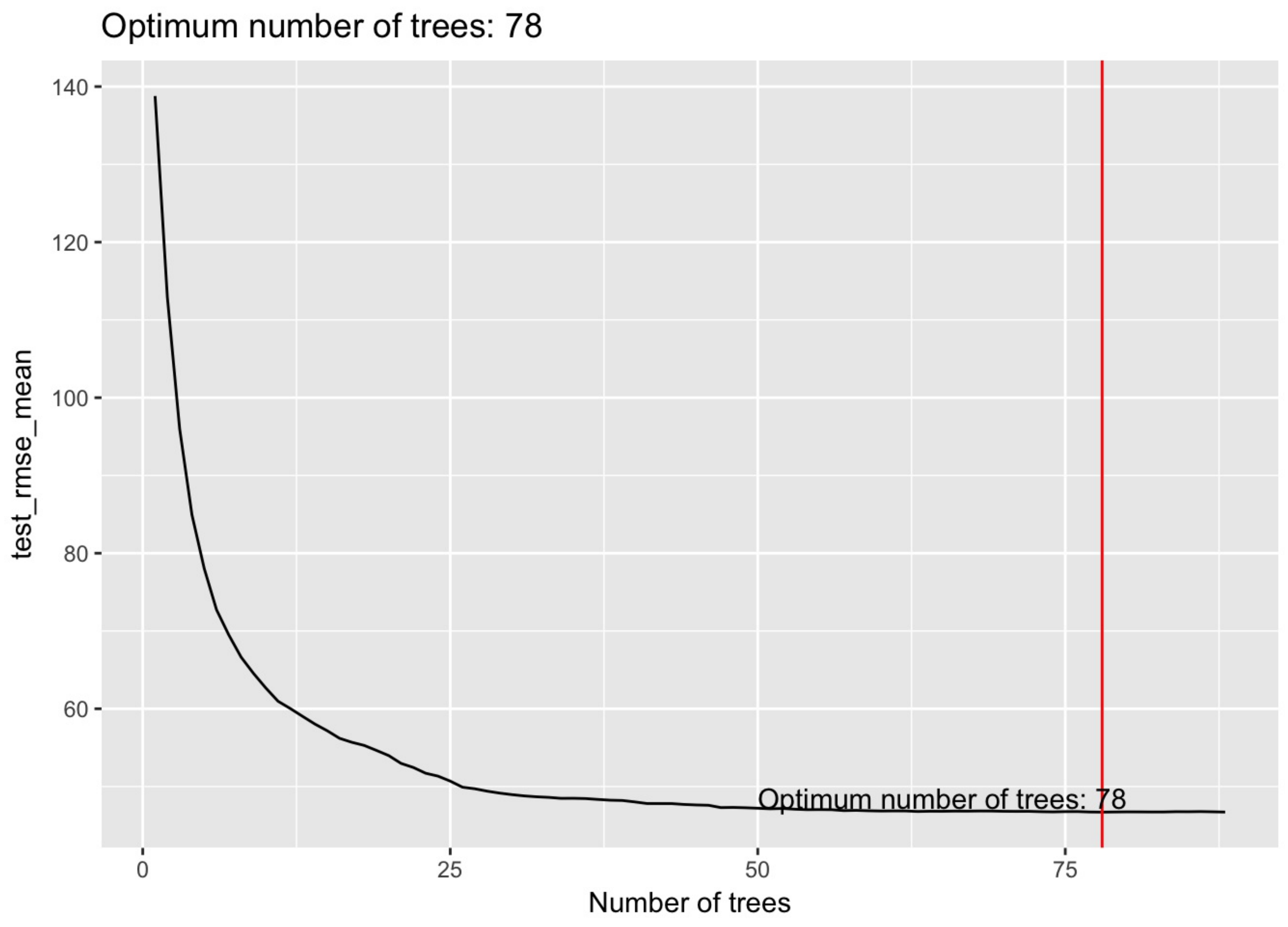
Training a model with xgboost() / xgb.cv()

```
> 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))
[1] 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

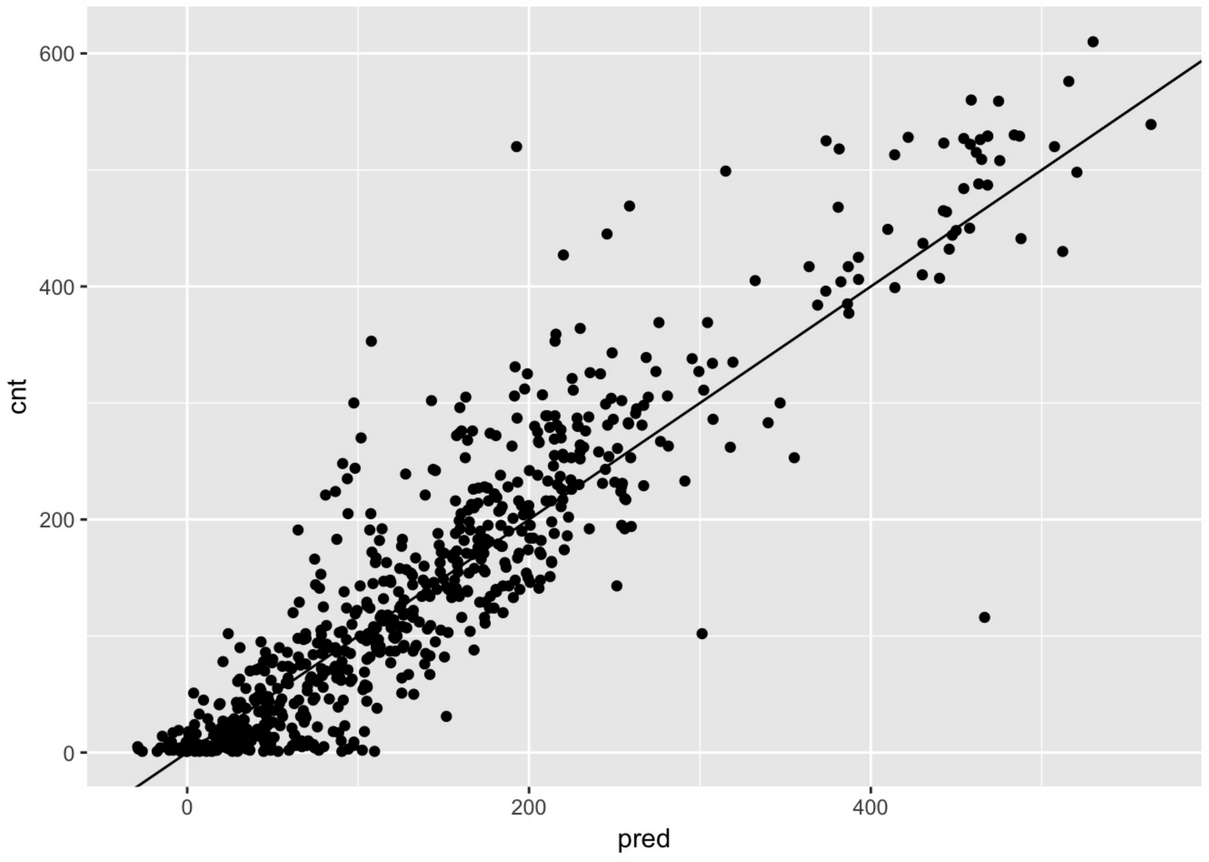
```
> bikesFeb.treat <- prepare(treatplan, bikesFeb, varRestriction = newvars)

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

Model performances on Febrary Data

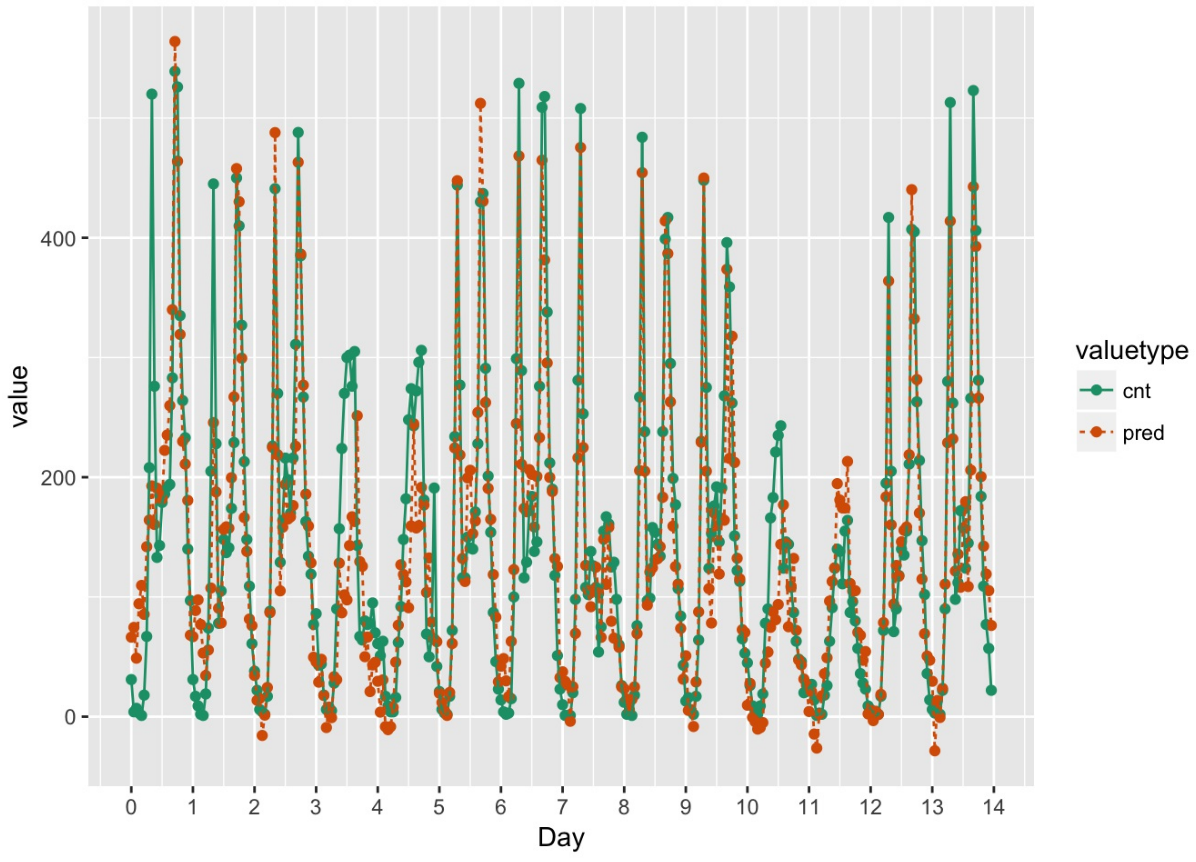
Model	RMSE
Quasipoisson	69.3
Random forests	67.15
Gradient Boosting	**54.0**

Visualize the Results

Predictions vs. Actual Bike Rentals, February



Predictions and Hourly Bike Rentals, February



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