



SUPERVISED LEARNING IN R: REGRESSION

# **Logistic regression to predict probabilities**

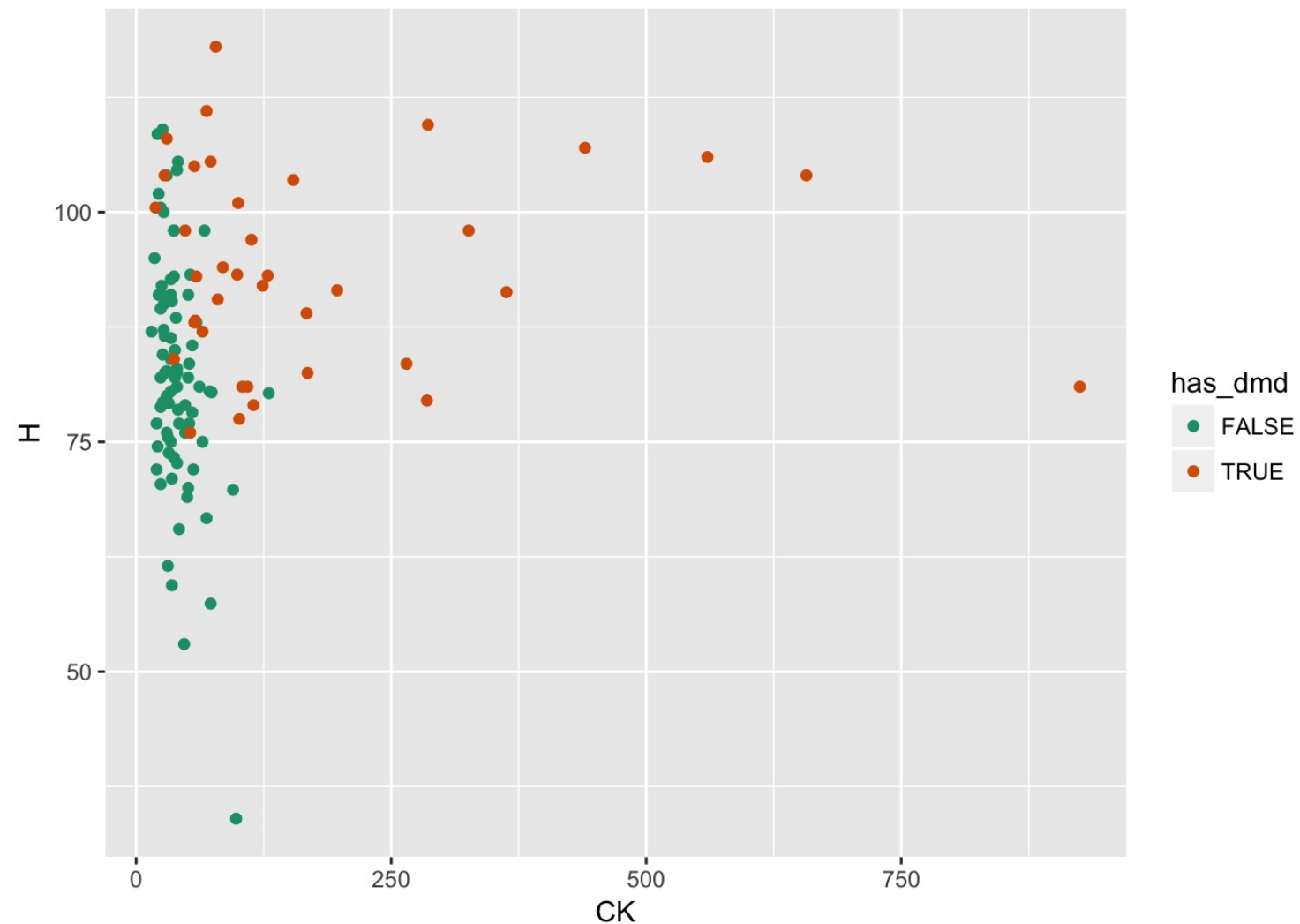
Nina Zumel and John Mount  
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# Predicting Probabilities

- Predicting *whether* an event occurs (yes/no): **classification**
- Predicting *the probability* that an event occurs: **regression**
- Linear regression: predicts values in  $[-\infty, \infty]$
- Probabilities: limited to  $[0,1]$  interval
  - So we'll call it non-linear

# Example: Predicting Duchenne Muscular Dystrophy (DMD)



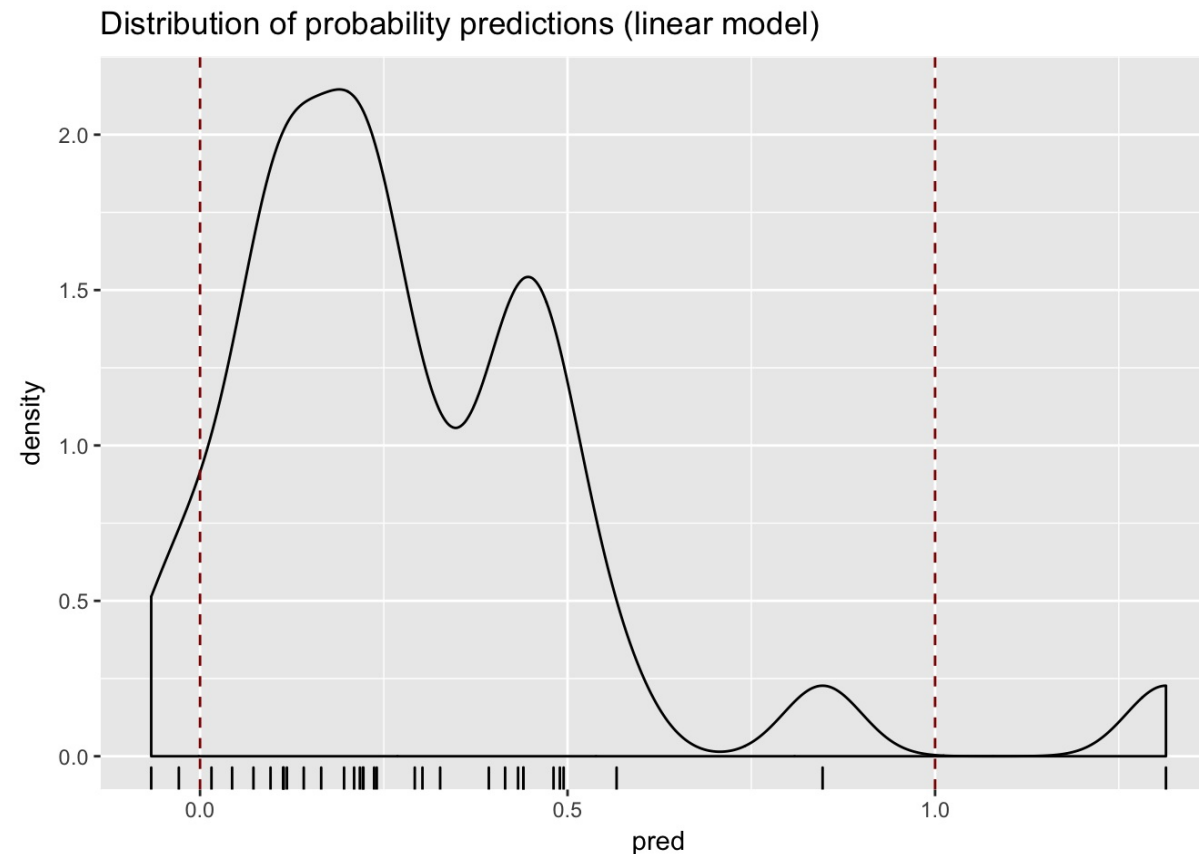
- outcome: has\_dmd
- inputs: CK, H

# A Linear Regression Model

```
model <- lm(has_dmd ~ CK + H,  
            data=train)  
  
test$pred <- predict(model,  
                    newdata = test)
```

- outcome:  $\text{has\_dmd} \in \{0,1\}$ 
  - 0: FALSE
  - 1: TRUE

**Model predicts values outside the range [0:1]**





# Logistic Regression

$$\log\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots$$

```
glm(formula, data, family = binomial)
```

- Generalized linear model
- Assumes inputs additive, linear in *log-odds*:  $\log(p/(1-p))$
- family: describes error distribution of the model
  - logistic regression: *family = binomial*



# DMD model

```
model <- glm(has_dmd ~ CK + H, data = train, family = binomial)
```

- outcome: two classes, e.g.  $a$  and  $b$
- model returns  $Prob(b)$ 
  - Recommend: 0/1 or FALSE/TRUE



# Interpreting Logistic Regression Models

```
model
```

```
## Call: glm(formula = has_dmd ~ CK + H, family = binomial, data = train)
```

```
##
```

```
## Coefficients:
```

```
## (Intercept)      CK      H
```

```
## -16.22046    0.07128    0.12552
```

```
##
```

```
## Degrees of Freedom: 86 Total (i.e. Null); 84 Residual
```

```
## Null Deviance:    110.8
```

```
## Residual Deviance: 45.16    AIC: 51.16
```



# Predicting with a glm() model

```
predict(model, newdata, type = "response")
```

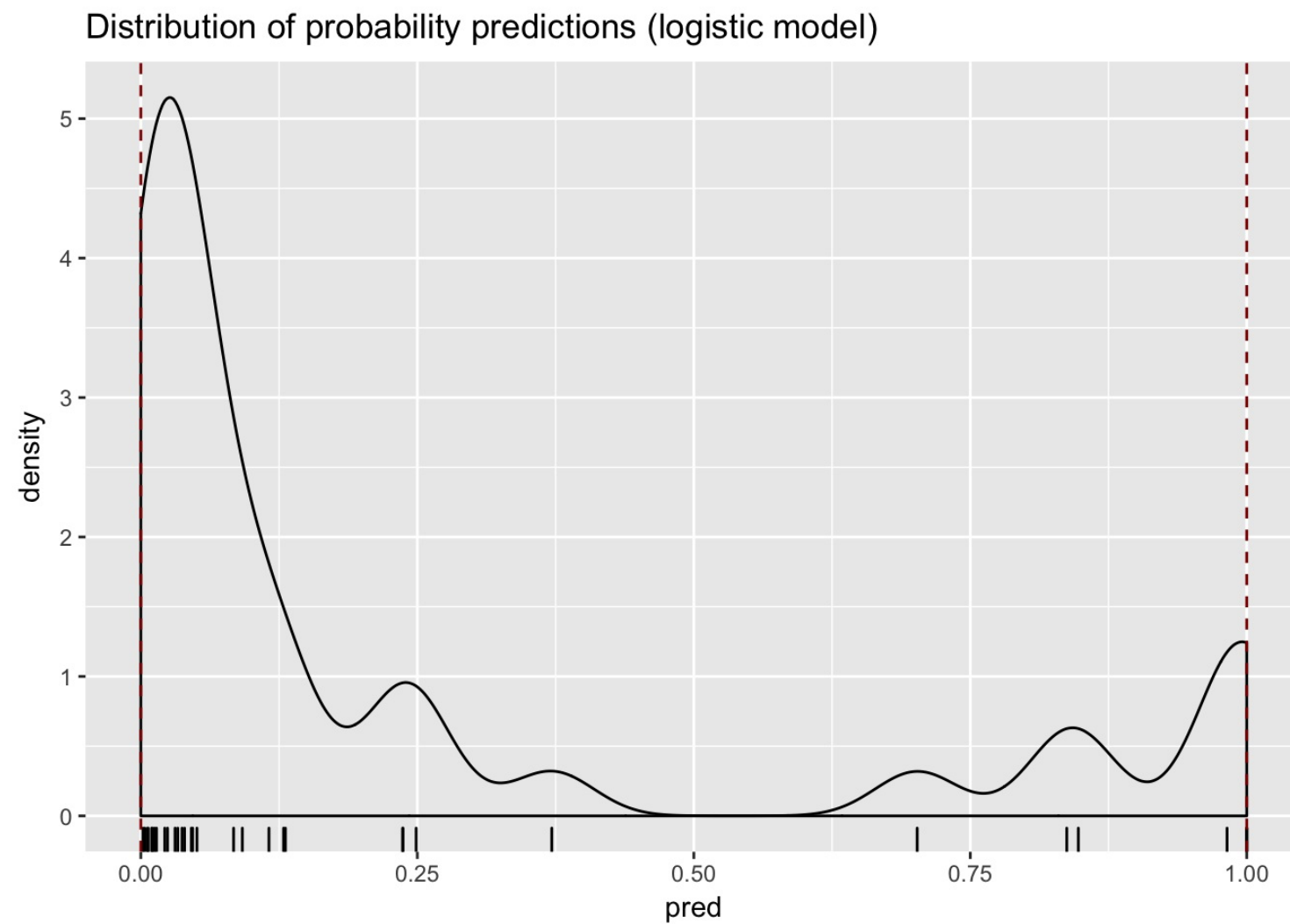
- newdata: by default, training data
- To get probabilities: use **type = "response"**
  - By default: returns log-odds





# DMD Model

```
model <- glm(has_dmd ~ CK + H, data = train, family = binomial)
test$pred <- predict(model, newdata = test, type = "response")
```





# Evaluating a logistic regression model: pseudo- $R^2$

$$R^2 = 1 - \frac{RSS}{SS_{Tot}}$$

$$pseudoR^2 = 1 - \frac{deviance}{null.deviance}$$

- Deviance: analogous to variance (RSS)
- Null deviance: Similar to  $SS_{Tot}$
- pseudo  $R^2$ : Deviance explained



# Pseudo- $R^2$ on Training data

Using `broom::glance()`

```
glance(model) %>%  
  summarize(pR2 = 1 - deviance/null.deviance)  
  
##    pseudoR2  
## 1 0.5922402
```

Using `sigr::wrapChiSqTest()`

```
wrapChiSqTest(model)  
  
## "... pseudo-R2=0.59 ..."
```

# Pseudo- $R^2$ on Test data

```
# Test data
test %>%
  mutate(pred = predict(model, newdata = test, type = "response")) %>%
  wrapChiSqTest("pred", "has_dmd", TRUE)
```

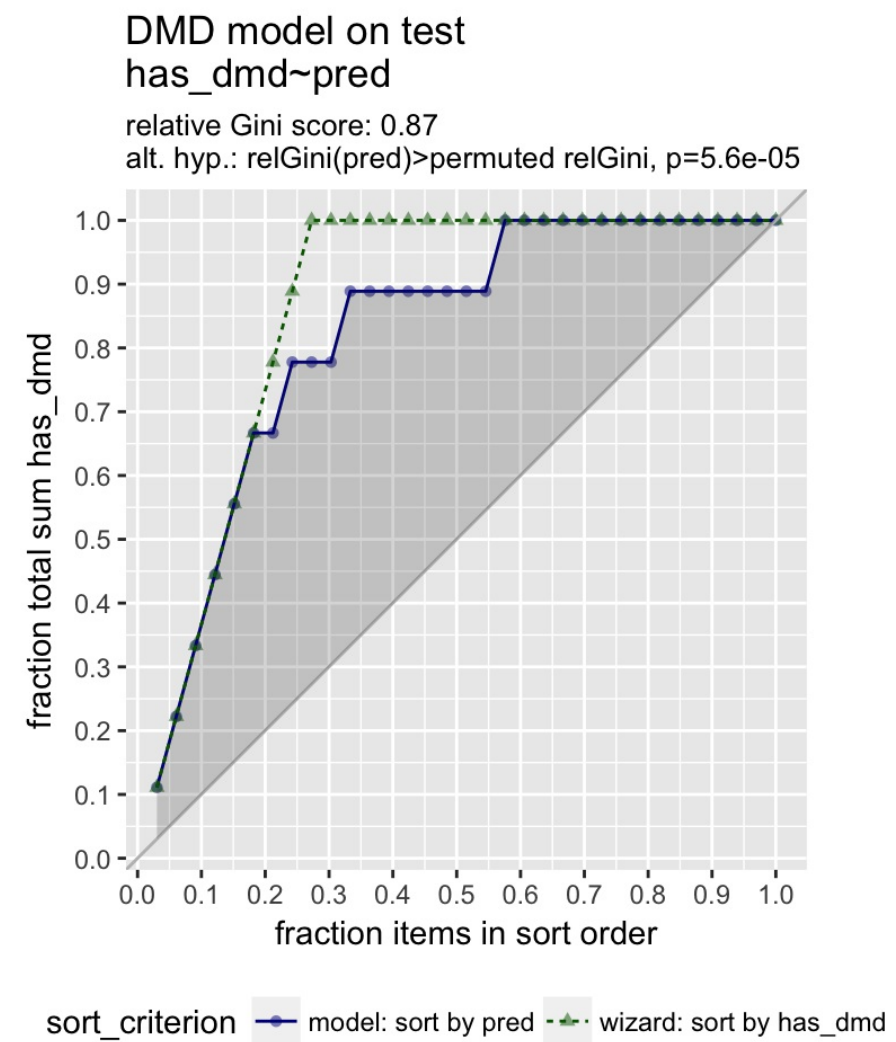
## Arguments:

- data frame
- prediction column name
- outcome column name
- target value (target event)



# The Gain Curve Plot

```
GainCurvePlot(test, "pred", "has_dmd", "DMD model on test")
```





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**Let's practice!**



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# **Poisson and quasipoisson regression to predict counts**

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Win-Vector, LLC



# Predicting Counts

- Linear regression: predicts values in  $[-\infty, \infty]$
- Counts: integers in range  $[0, \infty]$





# Poisson/Quasipoisson Regression

```
glm(formula, data, family)
```

- family: either poisson or quasipoisson
- inputs additive and linear in  $\log(\text{count})$

# Poisson/Quasipoisson Regression

```
glm(formula, data, family)
```

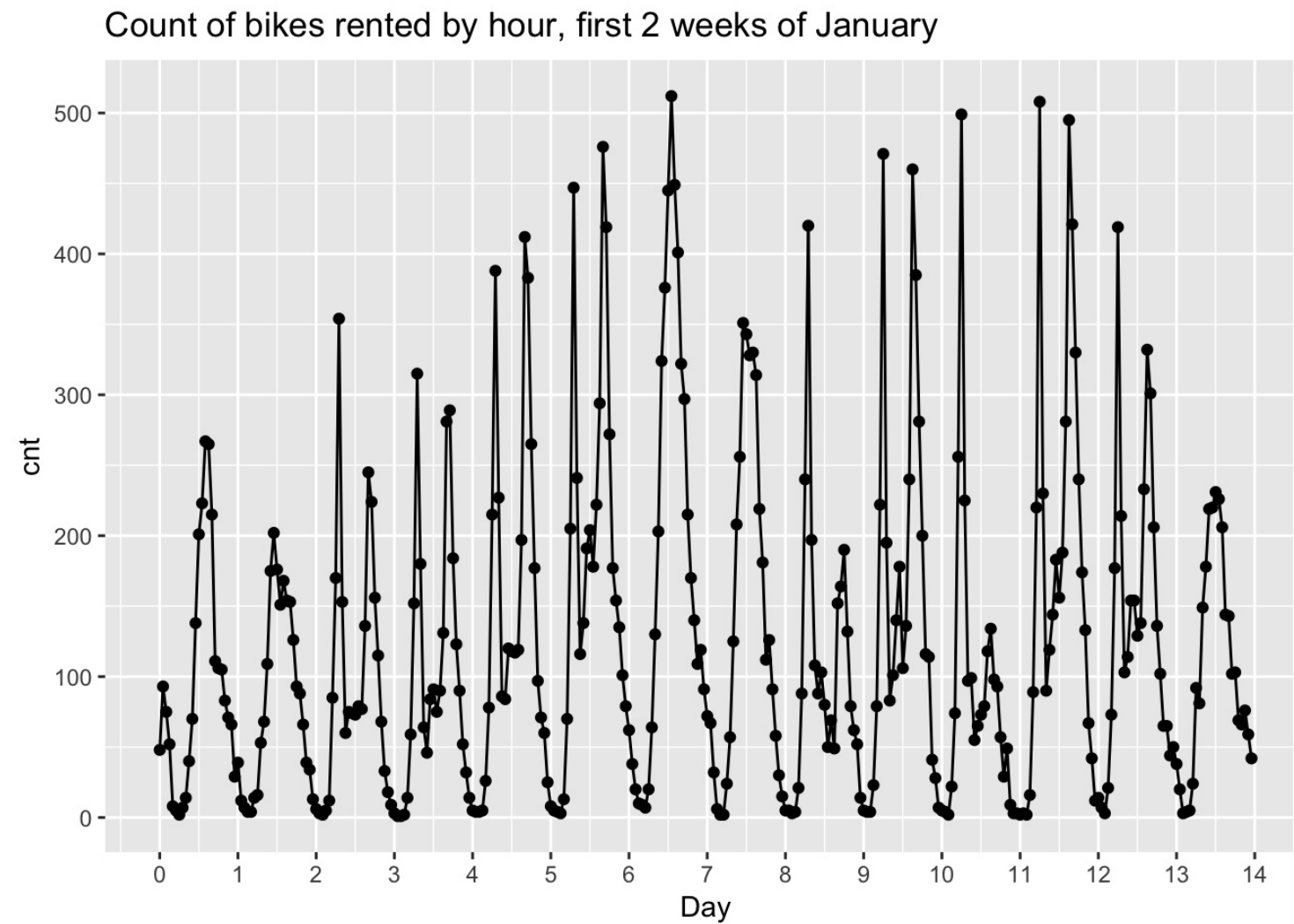
- family: either poisson or quasipoisson
- inputs additive and linear in  $\log(\text{count})$
- outcome: *integer*
  - counts: e.g. number of traffic tickets a driver gets
  - rates: e.g. number of website hits/day
- prediction: expected *rate* or *intensity* (not integral)
  - expected # traffic tickets; expected hits/day



# Poisson vs. Quasipoisson

- Poisson assumes that  $\text{mean}(y) = \text{var}(y)$
- If  $\text{var}(y)$  much different from  $\text{mean}(y)$  - quasipoisson
- Generally requires a large sample size
- If rates/counts  $\gg 0$  - regular regression is fine

# Example: Predicting Bike Rentals





# Fit the model

```
summarize(bikesJan, mean = mean(cnt), var = var(cnt))
```

```
##      mean    var  
## 1 130.5587 14351.25
```

Since  $\text{var}(\text{cnt}) \gg \text{mean}(\text{cnt}) \rightarrow \textit{use quasipoisson}$

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

```
model <- glm(fmla, data = bikesJan, family = quasipoisson)
```



# Check model fit

$$pseudoR^2 = 1 - \frac{deviance}{null.deviance}$$

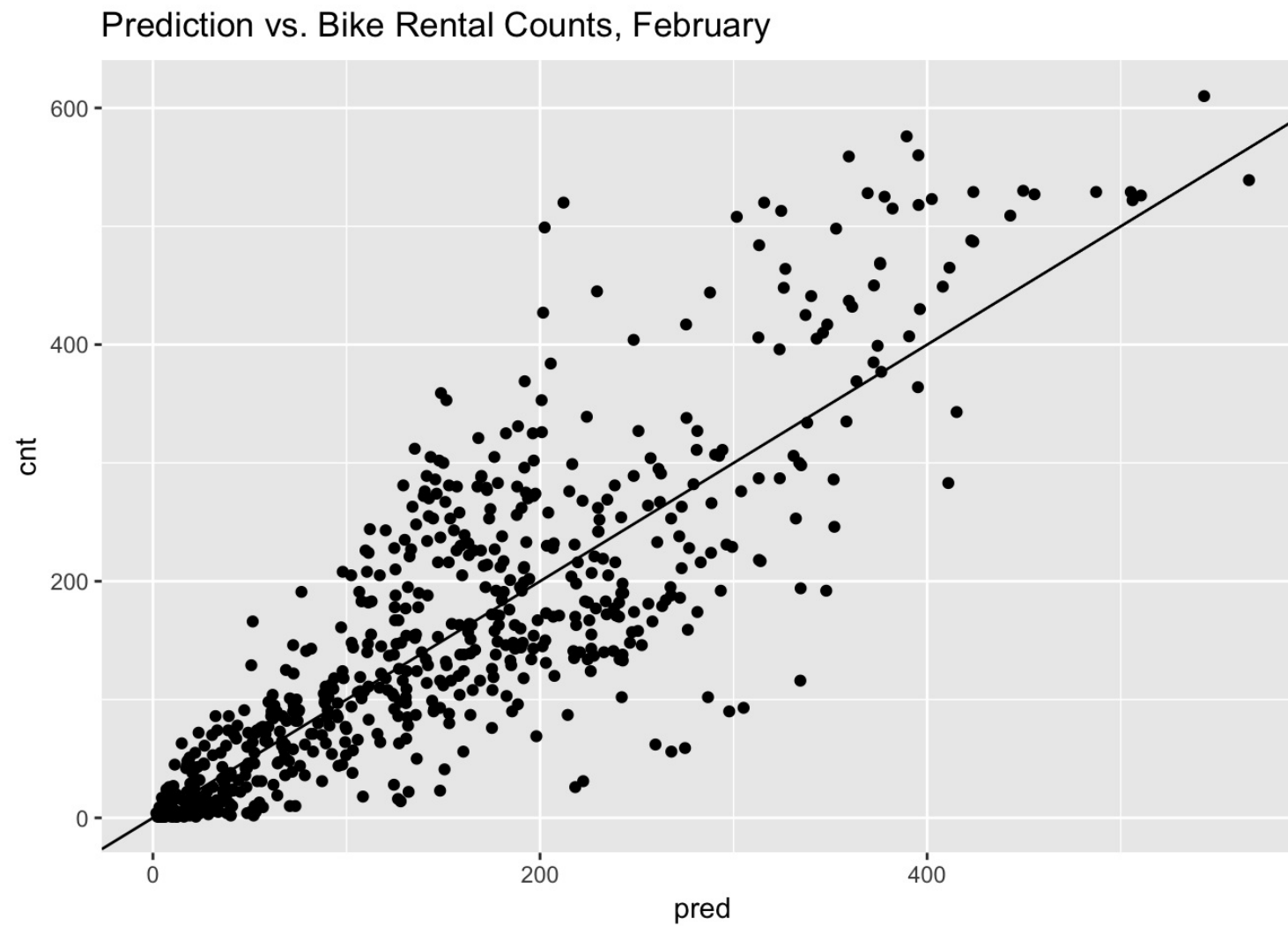
```
glance(model) %>%  
  summarize(pseudoR2 = 1 - deviance/null.deviance)
```

```
##    pseudoR2  
## 1 0.7654358
```



# Predicting from the model

```
predict(model, new data = bikesFeb, type = "response")
```





# Evaluate the model

You can evaluate count models by RMSE

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

```
##      rmse  
## 1 69.32869
```

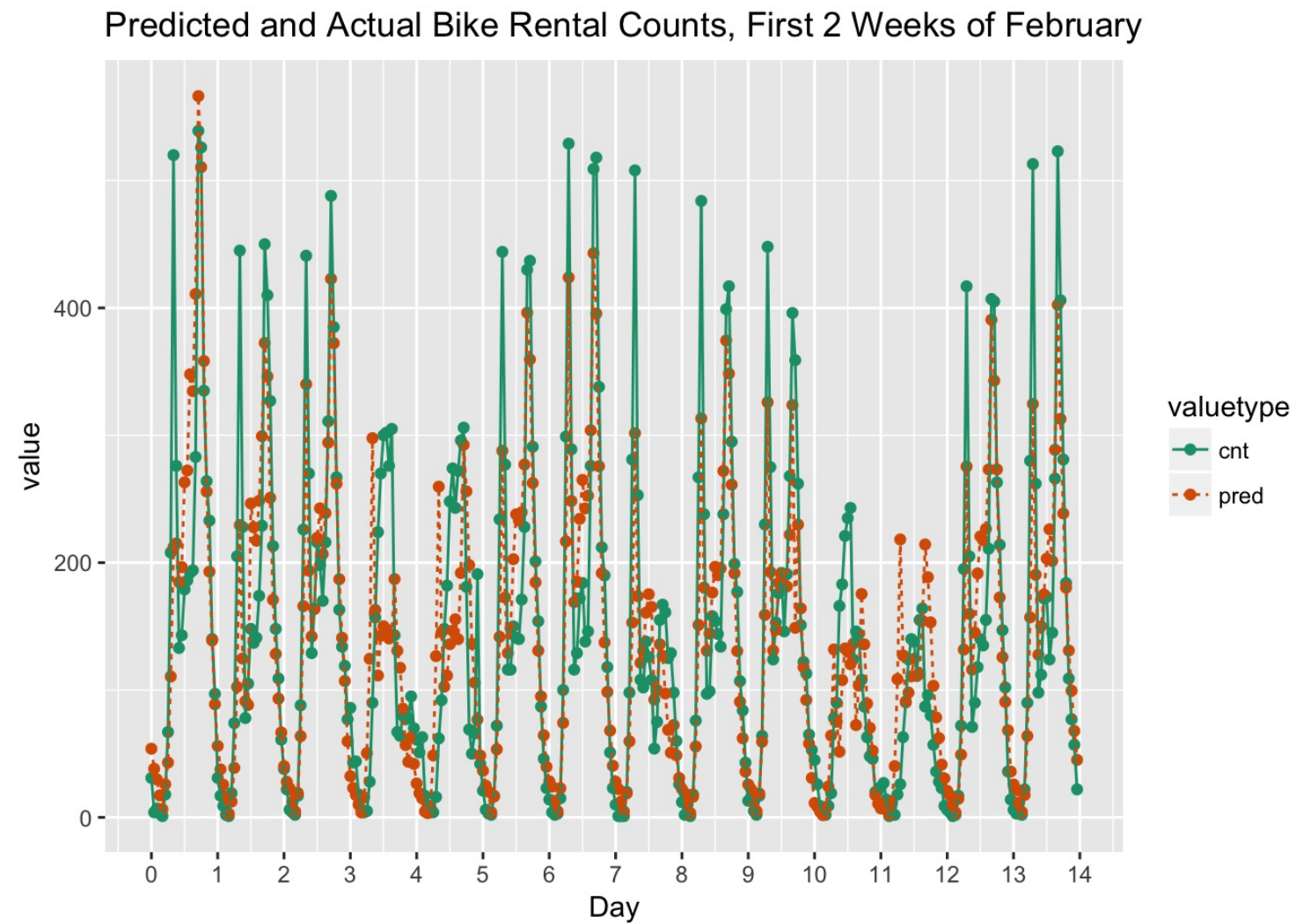
```
sd(bikesFeb$cnt)
```

```
## [1] 134.2865
```





# Compare Predictions and Actual Outcomes





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**Let's practice!**



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# **GAM to learn non-linear transformations**

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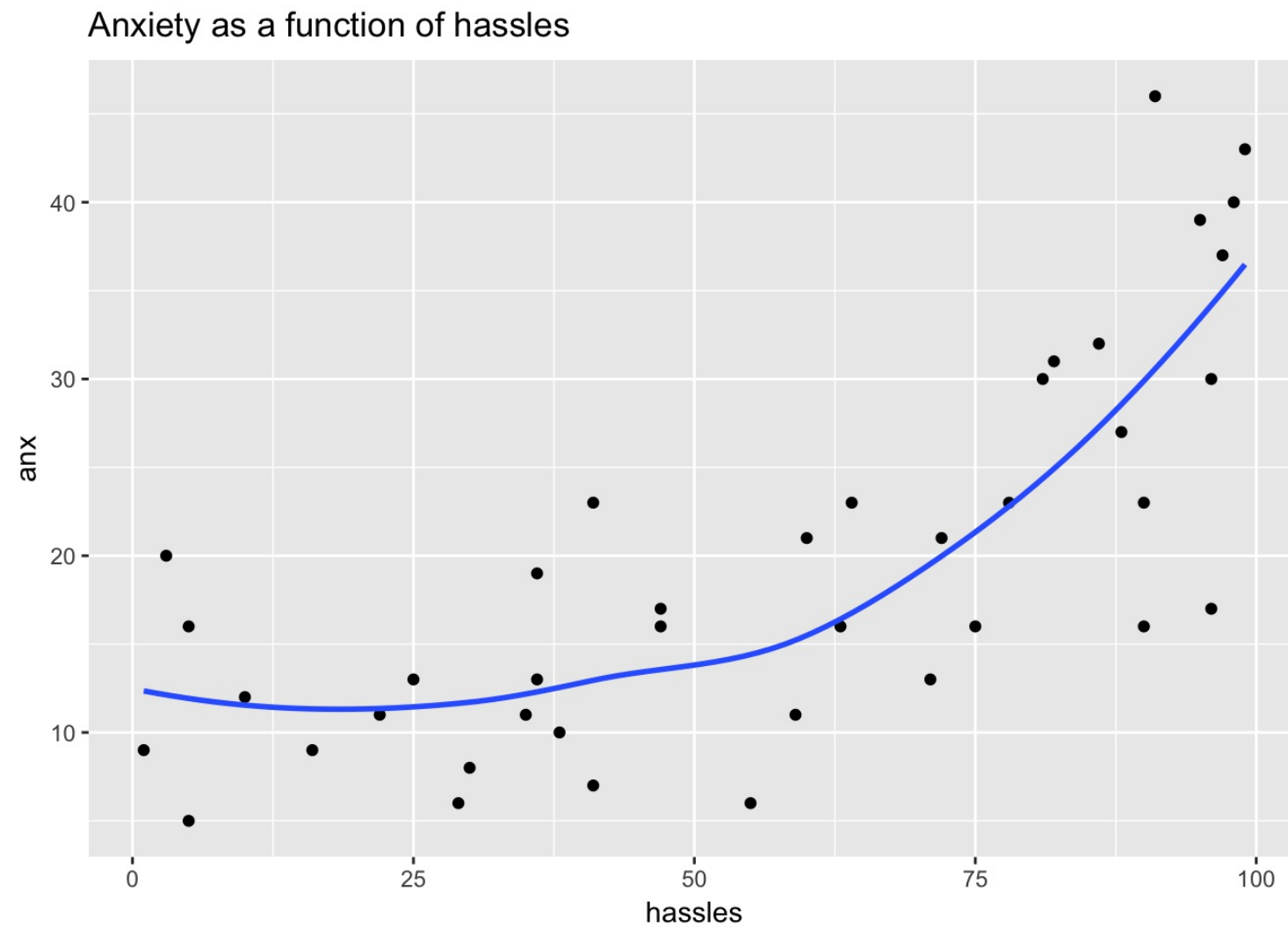


# Generalized Additive Models (GAMs)

$$y \sim b_0 + s_1(x_1) + s_2(x_2) + \dots$$



# Learning Non-linear Relationships





# gam() in the mgcv package

```
gam(formula, family, data)
```

family:

- gaussian (default): "regular" regression
- binomial: probabilities
- poisson/quasipoisson: counts

Best for larger data sets

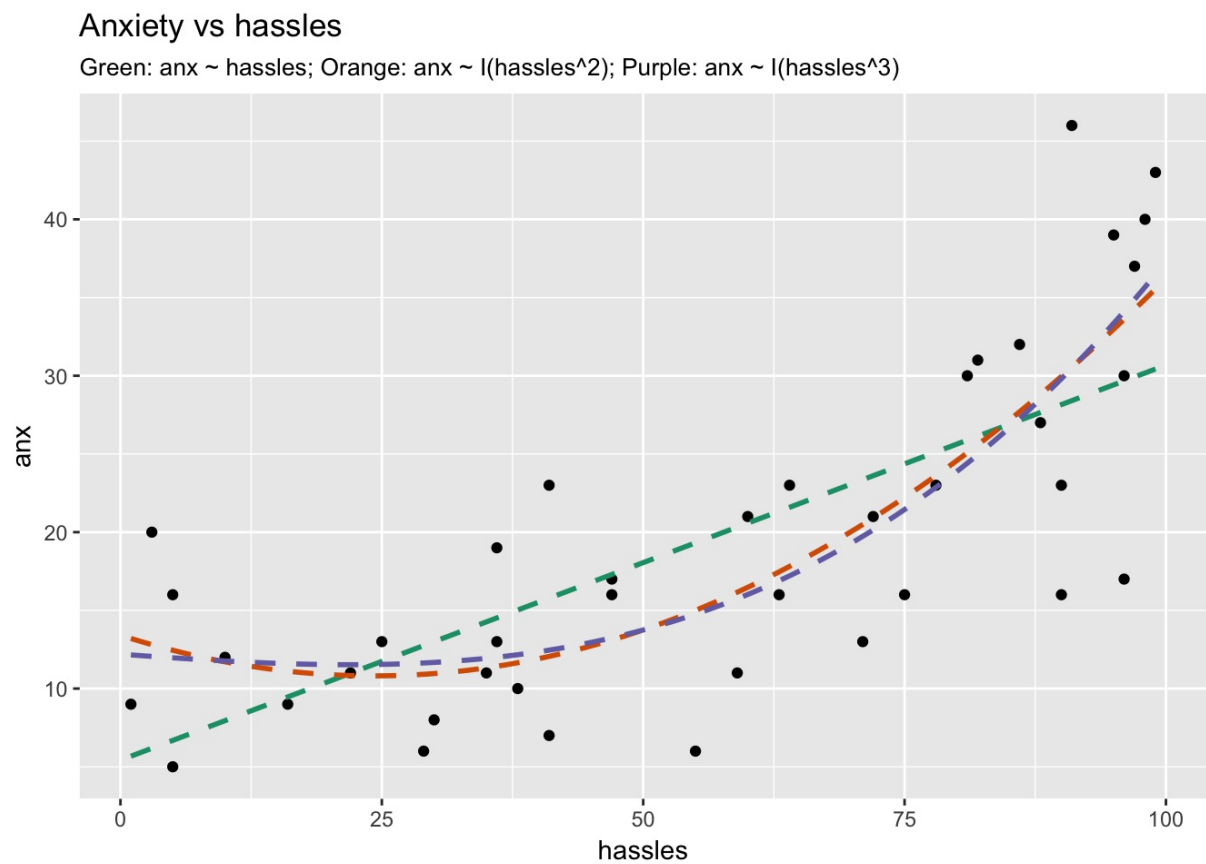


# The `s()` function

`anx ~ s(hassles)`

- `s()` designates that variable should be non-linear
- Use `s()` with continuous variables
  - More than about 10 unique values

# Revisit the hassles data



Model	RMSE (cross-val)	$R^2$ (training)
Linear ( <i>hassles</i> )	7.69	0.53
Quadratic ( <i>hassles</i> <sup>2</sup> )	6.89	0.63
<b>Cubic (</b> <i>hassles</i> <sup>3</sup> )	<b>6.70</b>	<b>0.65</b>





# GAM of the hassles data

```
model <- gam(anx ~ s(hassles), data = hassleframe, family = gaussian)
```

```
summary(model)
```

```
##
```

```
## ...
```

```
##
```

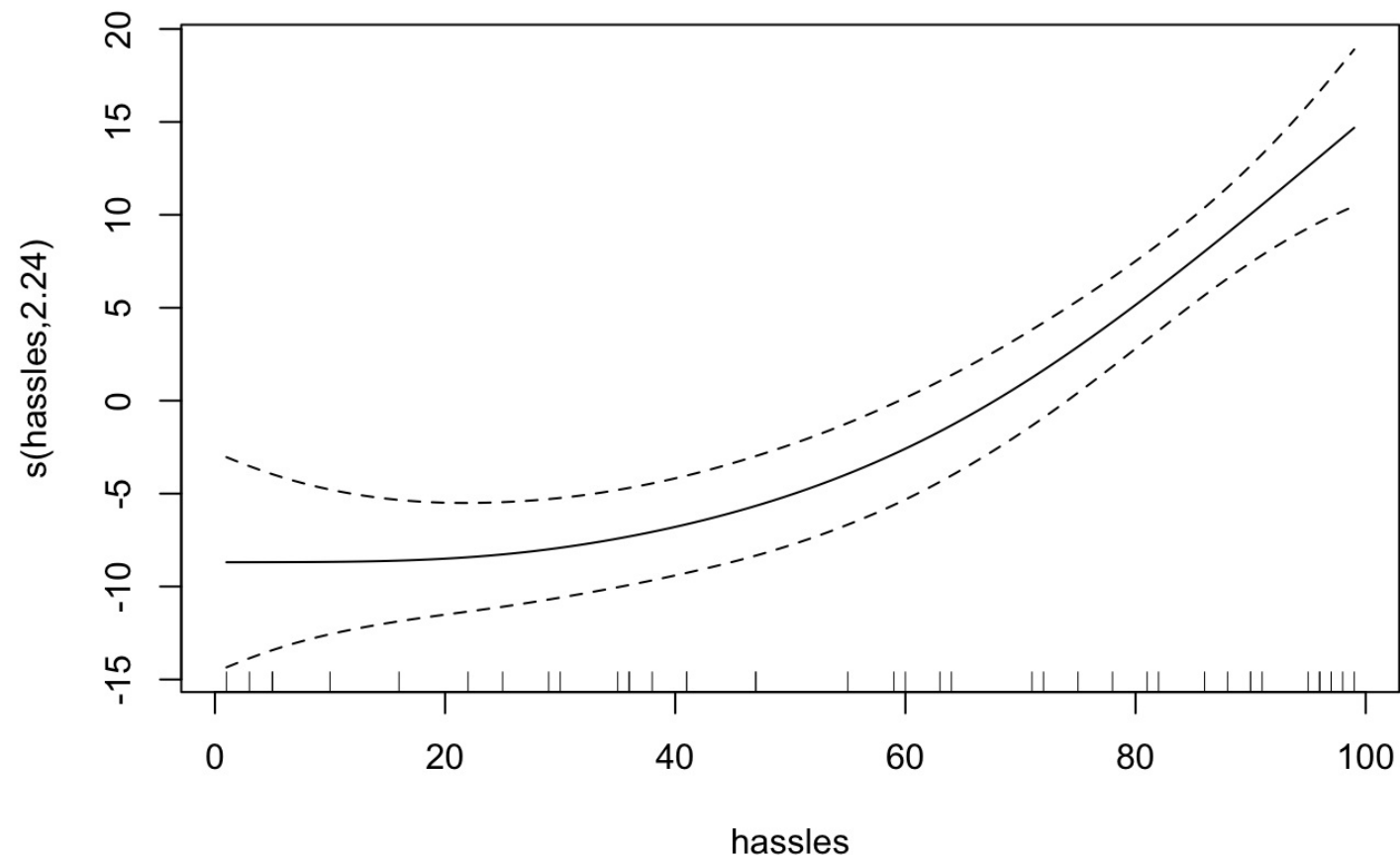
```
## R-sq.(adj) = 0.619  Deviance explained = 64.1%
```

```
## GCV = 49.132  Scale est. = 45.153  n = 40
```



# Examining the Transformations

```
plot(model)
```

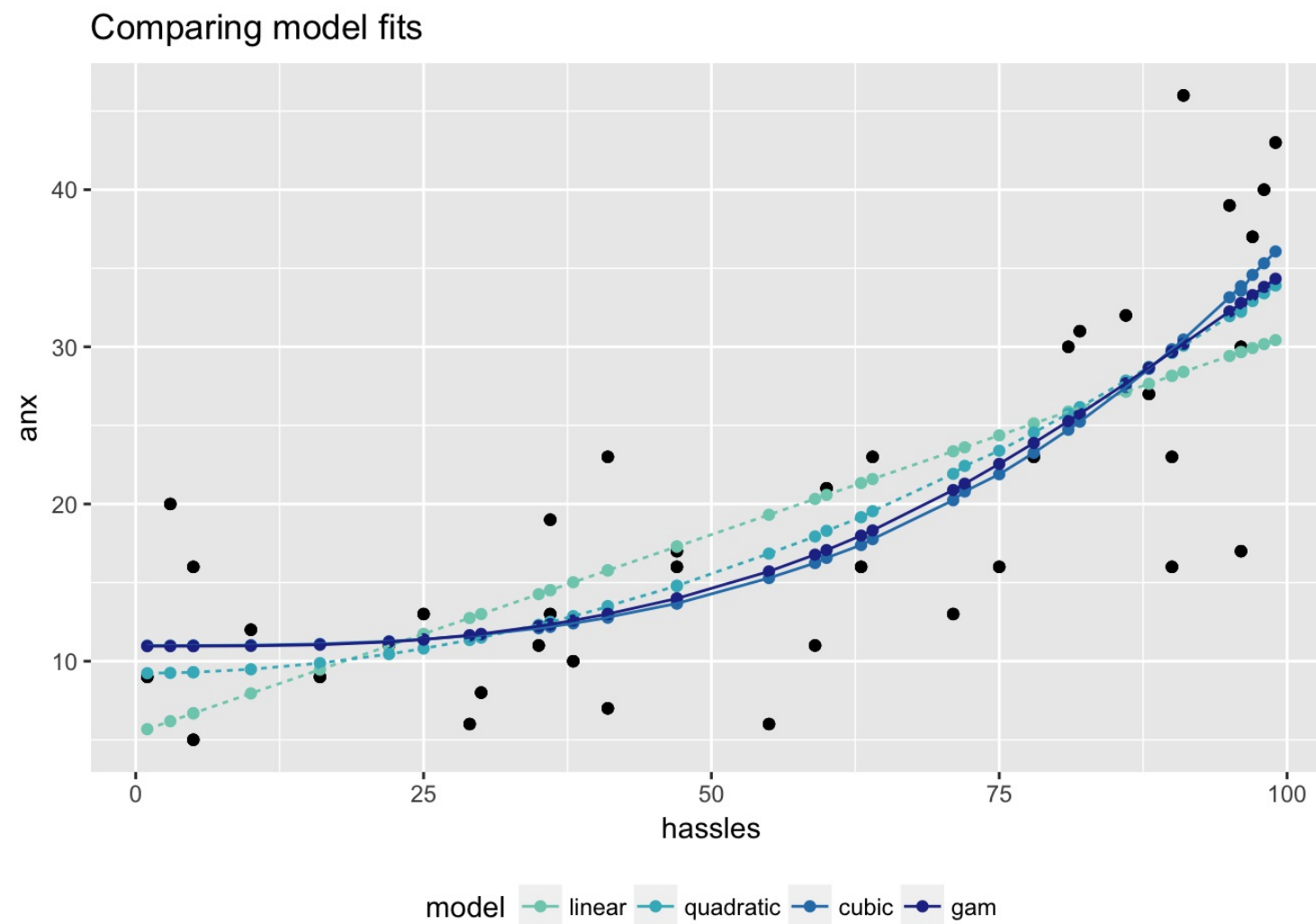


$y$  values: `predict(model, type = "terms")`



# Predicting with the Model

```
predict(model, newdata = hassleframe, type = "response")
```



# Comparing out-of-sample performance

Knowing the correct transformation is best, but GAM is useful when transformation isn't known

Model	RMSE (cross-val)	$R^2$ (training)
Linear ( <i>hassles</i> )	7.69	0.53
Quadratic ( <i>hassles</i> <sup>2</sup> )	6.89	0.63
Cubic ( <i>hassles</i> <sup>3</sup> )	6.70	0.65
GAM	<b>7.06</b>	0.64

- Small data set → noisier GAM



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