



SUPERVISED LEARNING IN R: REGRESSION

# Logistic regression to predict probabilities

Nina Zumel and John Mount Win-Vector LLC

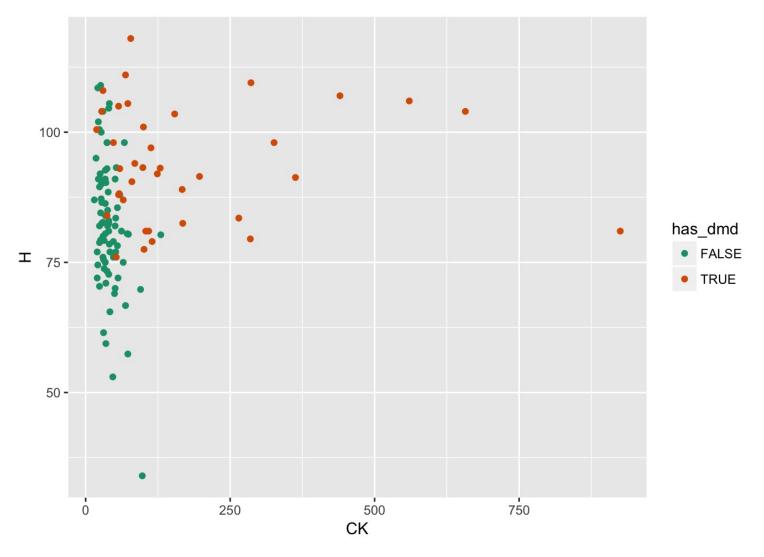


# Predicting Probabilities

- 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



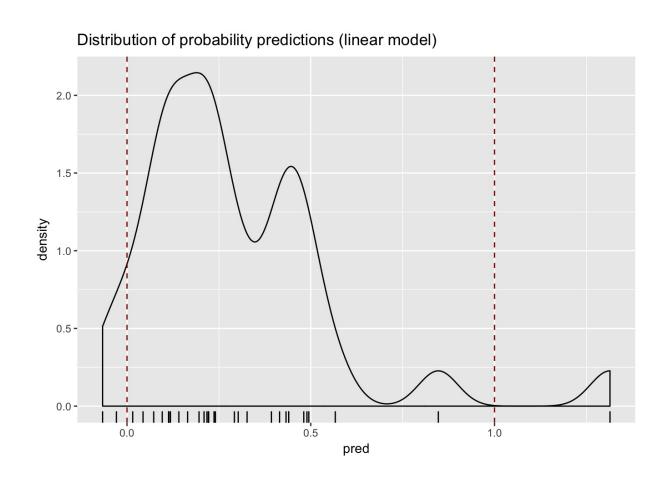
## A Linear Regression Model

• outcome: has\_dmd  $\in \{0,1\}$ 

• 0: FALSE

■ 1: TRUE

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





# Logistic Regression

$$log(rac{p}{1-p})=eta_0+eta_1x_1+eta_2x_2+...$$

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)</pre>
```

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



## Interpreting Logistic Regression Models



# Predicting with a glm() model

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

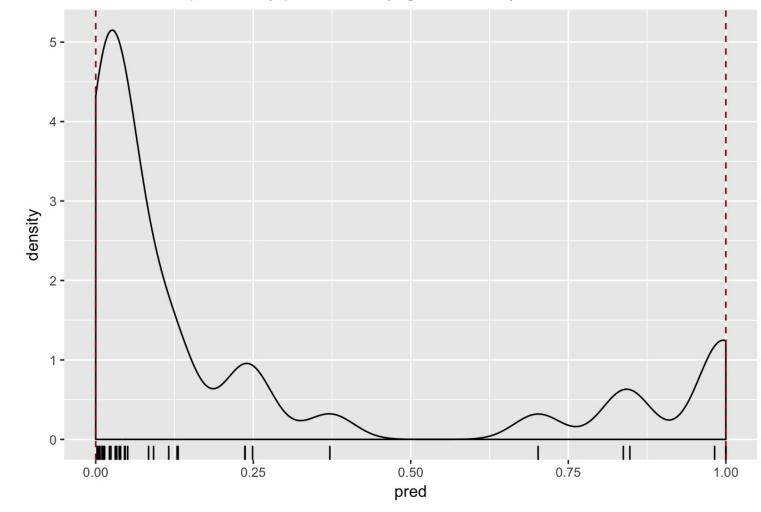
- newdata: by default, training data
- To get probabilities: use type = "response"
  - By default: returns log-odds



#### DMD Model

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

#### Distribution of probability predictions (logistic model)





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

$$R^2 = 1 - rac{RSS}{SS_{Tot}}$$
  $pseudoR^2 = 1 - rac{deviance}{null.deviance}$ 

- 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)
```

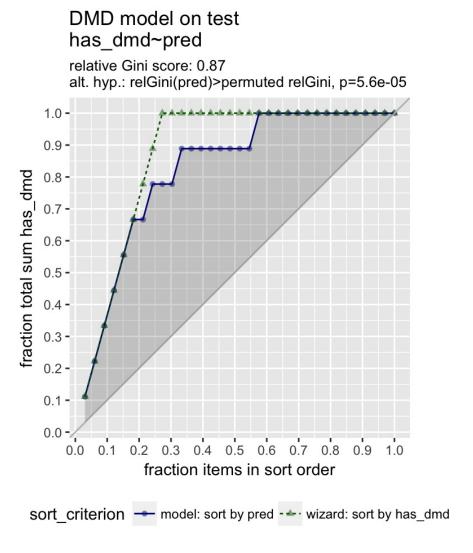
#### Arguments:

- 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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# **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(count)

# Poisson/Quasipoisson Regression

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

- family: either poisson or quasipoisson
- inputs additive and linear in log(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

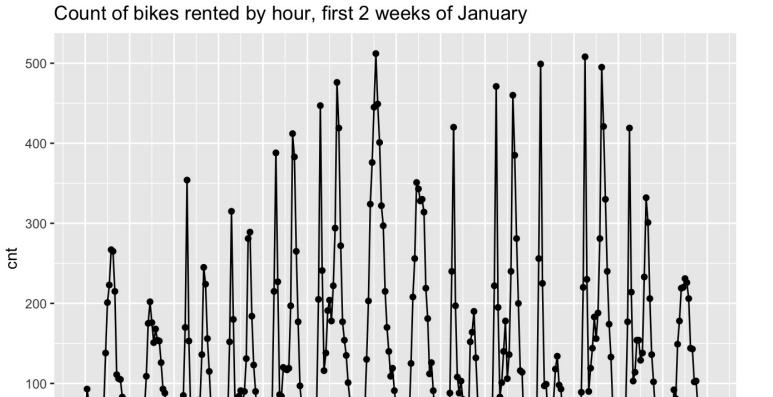


# Poisson vs. Quasipoisson

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



# Example: Predicting Bike Rentals



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#### Fit the model

```
> bikesJan %>%
+    summarize(mean = mean(cnt), var = var(cnt))
##    mean    var
## 1 130.5587 14351.25
```

#### Since var(cnt) >> mean(cnt) → use quasipoisson



#### Check model fit

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

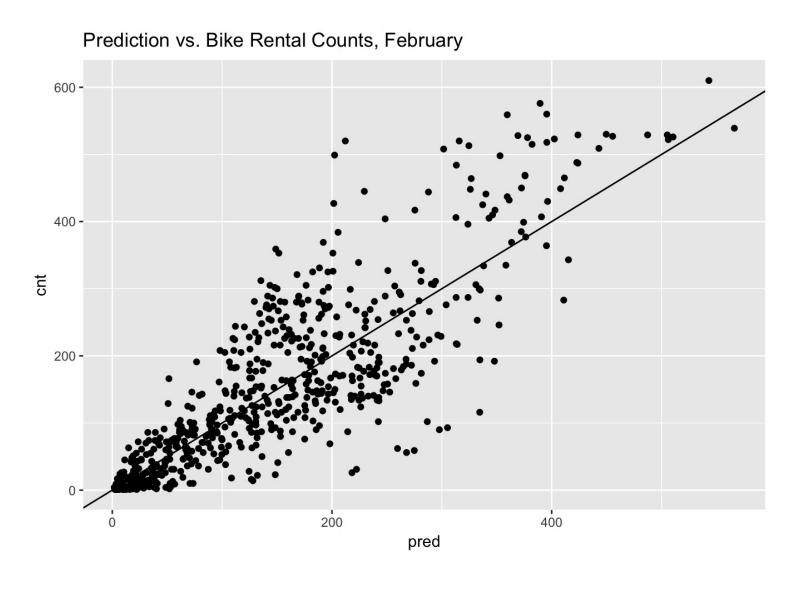
```
> glance(model) %>%
+ summarize(pseudoR2 = 1 - deviance/null.deviance)

## pseudoR2
## 1 0.7654358
```



# Predicting from the model

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





#### Evaluate the model

You can evaluate count models by RMSE

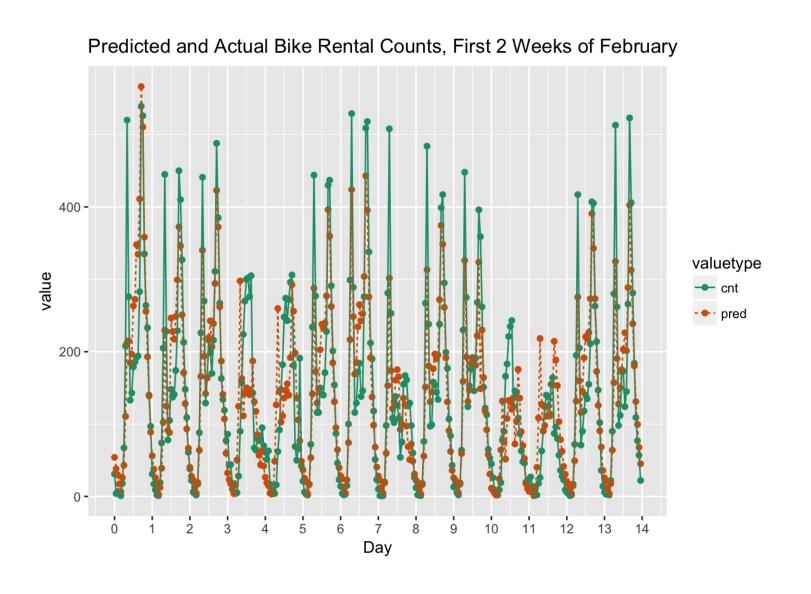
```
> bikesFeb %>%
+    mutate(residual = pred - cnt) %>%
+    summarize(rmse = sqrt(mean(residual^2)))

##    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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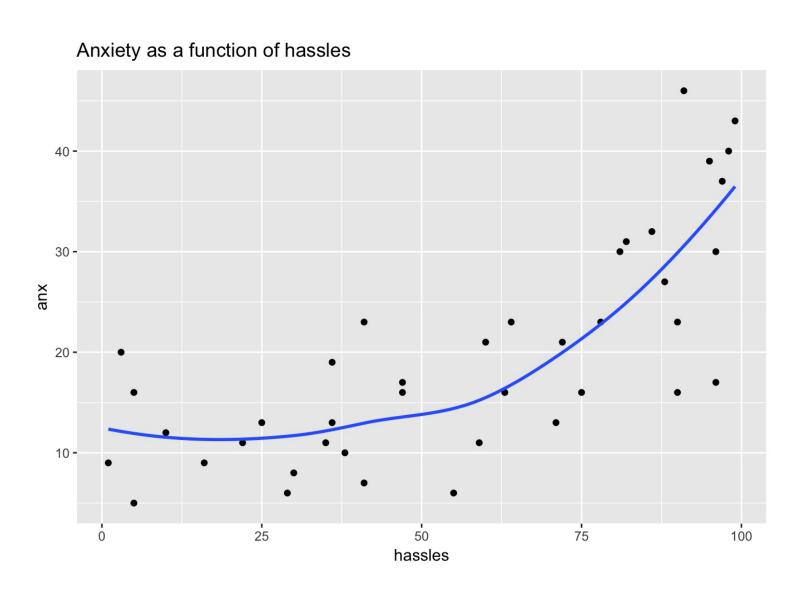


## Generalized Additive Models (GAMs)

$$y \sim b0 + s1(x1) + s2(x2) + ....$$



# 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

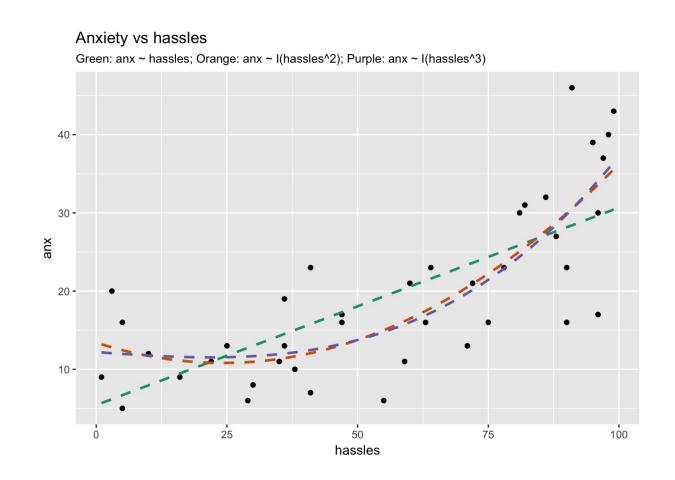
# The s() function

```
> 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 (  hassles)	7.69	0.53
Quadratic $(hassles^2)$	6.89	0.63
Cubic ( $hassles^3$ )	6.70	0.65



#### GAM of the hassles data

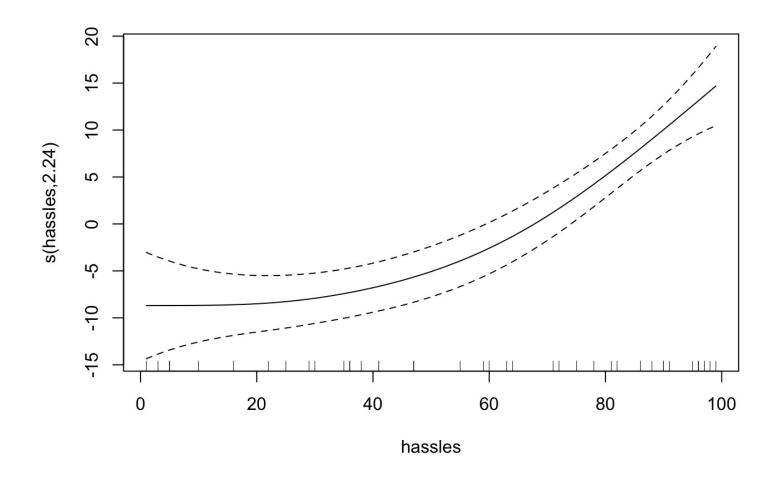
```
> model <- gam(anx ~ s(hassles), data = hassleframe, family = gaussian)
> summary(model)

## ...
##
## R-sq.(adj) = 0.619 Deviance explained = 64.1%
## GCV = 49.132 Scale est. = 45.153 n = 40
```



# Examining the Transformations

> plot(model)

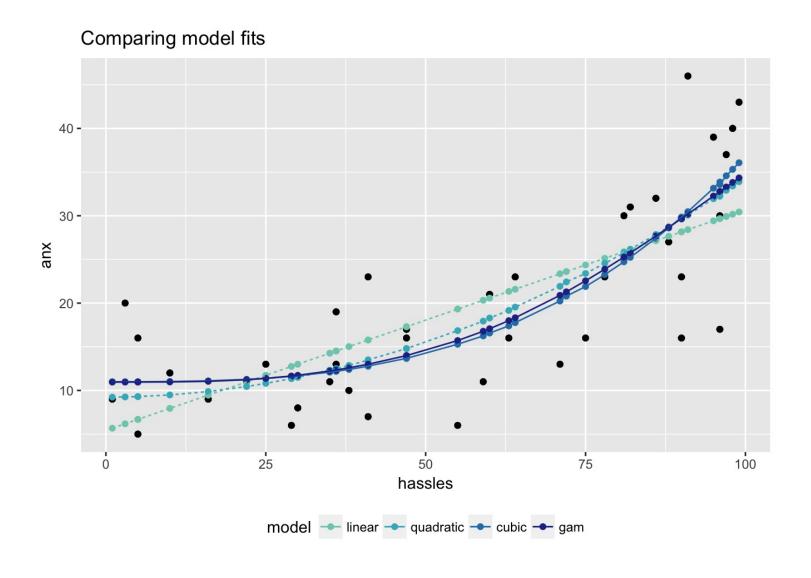


y values: predict(model, type = "terms")



# 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 (hassles)	7.69	0.53
Quadratic ( $hassles^2$ )	6.89	0.63
Cubic ( $hassles^3$ )	6.70	0.65
GAM	7.06	0.64

Small data set → noisier GAM





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# Let's practice!