



SUPERVISED LEARNING IN R: REGRESSION

## **Categorical inputs**

Nina Zumel and John Mount Win-Vector, LLC



#### Example: Effect of Diet on Weight Loss

WtLoss24 ~ Diet + Age + BMI

Diet	Age	ВМІ	WtLoss24
Med	59	30.67	-6.7
Low-Carb	48	29.59	8.4
Low-Fat	52	32.9	6.3
Med	53	28.92	8.3
Low-Fat	47	30.20	6.3



#### model.matrix()

 $model.matrix(WtLoss24 \sim Diet + Age + BMI, data = diet)$ 

- All numerical values
- Converts categorical variable with N levels into N-1 indicator variables



#### Indicator Variables to Represent Categories

#### **Original Data**

Diet	Age	
Med	59	
Low-Carb	48	
Low-Fat	52	
Med	53	
Low-Fat	47	

#### **Model Matrix**

(Intercept)	DietLow- Fat	DietMed	
1	0	1	
1	0	0	
1	1	0	
1	0	1	
1	1	0	

reference level: "Low-Carb"



#### Interpreting the Indicator Variables

#### **Linear Model:**

```
WtLoss24 = \beta_0 + \beta_{DietLowFat} x_{DietLowFat} + \beta_{DietMed} x_{DietMed} + \beta_{Age} x_{Age} + \beta_{BMI} x_{BMI}
```

```
Im(WtLoss24 ~ Diet + Age + BMI, data=diet))
## Coefficients:
                     DietLow-Fat
##
       (Intercept)
                                   DietMed
         -1.37149
                                  -0.97883
##
                       -2.32130
##
           Age
                        BMI
         0.12648
                        0.01262
##
```



#### Issues with one-hot-encoding

- Too many levels can be a problem
  - Example: ZIP code (about 40,000 codes)
- Don't hash with geometric methods!





SUPERVISED LEARNING IN R: REGRESSION

# Let's practice!





SUPERVISED LEARNING IN R: REGRESSION

#### Interactions

Nina Zumel and John Mount Win-Vector, LLC



#### Additive relationships

Example of an additive relationship:

```
plant_height ~ bacteria + sun
```

- Change in height is the sum of the effects of bacteria and sunlight
- Change in sunlight causes same change in height, independent of bacteria
- Change in bacteria causes same change in height, independent of sunlight



#### What is an Interaction?

The simultaneous influence of two variables on the outcome is not additive.

```
plant_height ~ bacteria + sun + bacteria:sun
```

- Change in height is more (or less) than the sum of the effects due to sun/bacteria
- At higher levels of sunlight, 1 unit change in bacteria causes more change in height



#### What is an Interaction?

The simultaneous influence of two variables on the outcome is not additive.

```
plant_height ~ bacteria + sun + bacteria:sun
```

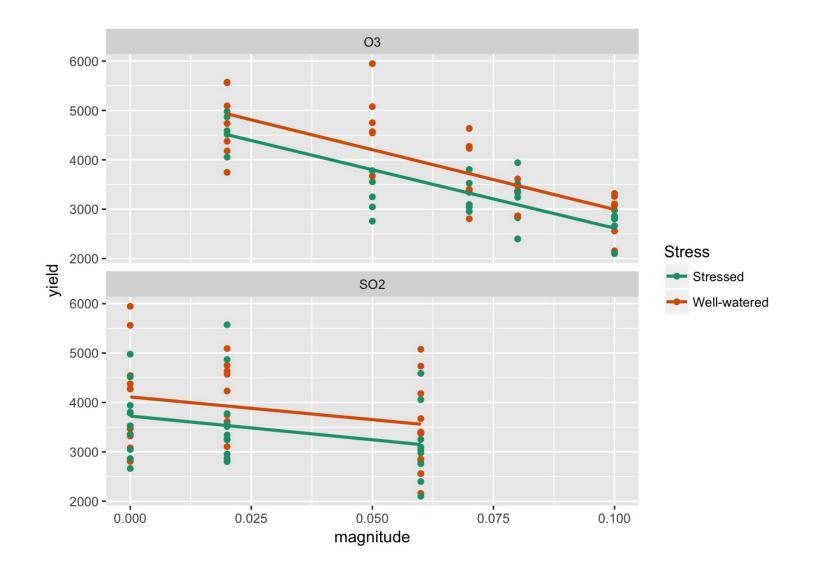
- sun: categorical {"sun", "shade"}
- In sun, 1 unit change in bacteria causes m units change in height
- In shade, 1 unit change in bacteria causes *n* units change in height

Like two separate models: one for sun, one for shade.



#### Example of No Interaction: Soybean Yield

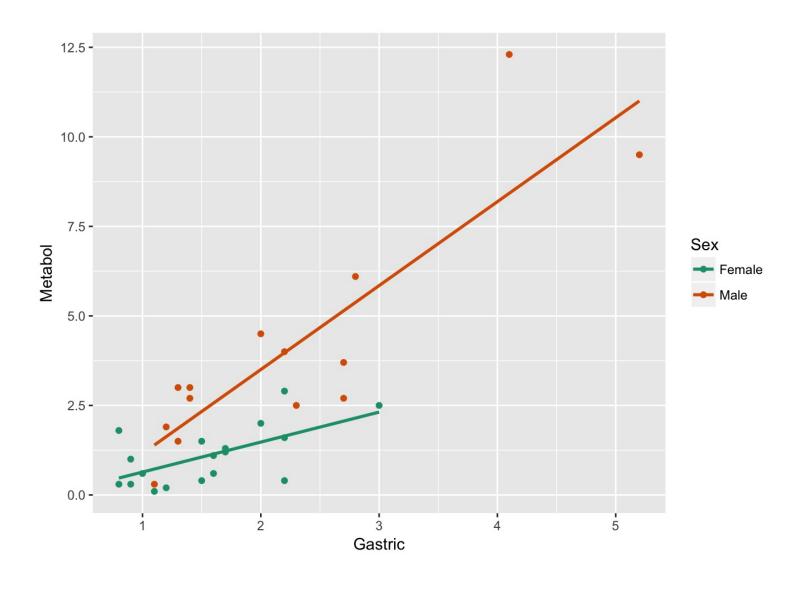
yield ~ Stress + SO2 + O3





#### Example of an Interaction: Alcohol Metabolism

Metabol ~ Gastric + Sex



#### Expressing Interactions in Formulae

• Interaction - Colon (:)

```
y ~ a:b
```

Main effects and interaction - Asterisk (\*)

```
y \sim a*b
# Both mean the same
y \sim a + b + a:b
```

Expressing the product of two variables - I

```
y \sim I(a*b)
```



#### Finding the Correct Interaction Pattern

Formula	RMSE (cross validation)
Metabol ~ Gastric + Sex	1.46
Metabol ~ Gastric * Sex	1.48
Metabol ~ Gastric + Gastric:Sex	1.39





SUPERVISED LEARNING IN R: REGRESSION

# Let's practice!





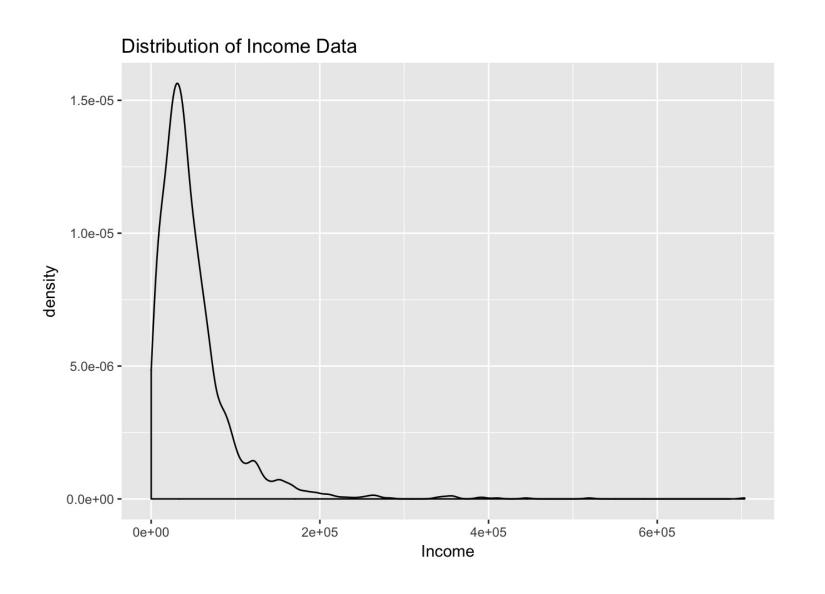
SUPERVISED LEARNING IN R: REGRESSION

# Transforming the response before modeling

Nina Zumel and John Mount Win-Vector, LLC



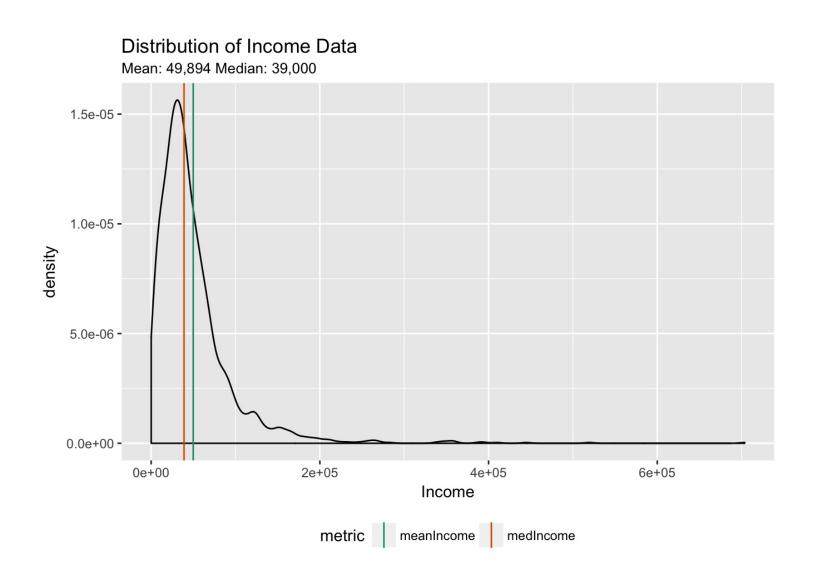
#### The Log Transform for Monetary Data



- Monetary values: lognormally distributed
- Long tail, wide dynamic range (60-700K)



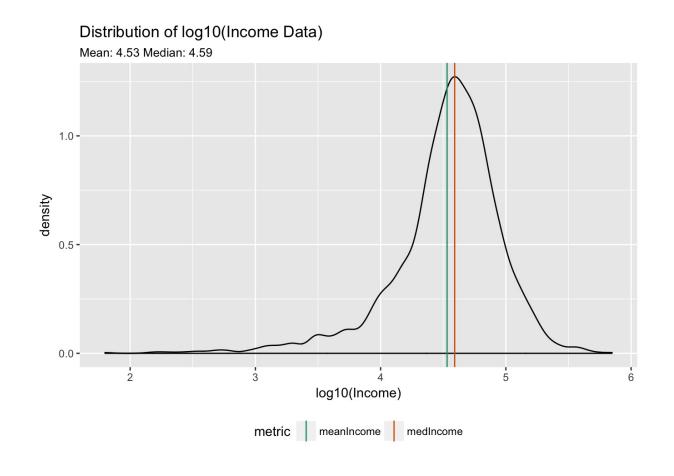
#### Lognormal Distributions



- mean > median (~ 50K vs 39K)
- Predicting the mean will overpredict typical values



#### Back to the Normal Distribution



For a Normal Distribution:

- mean = median (here: 4.53 vs4.59)
- more reasonable dynamic range
   (1.8 5.8)



#### The Procedure

1. Log the outcome and fit a model

```
model <- Im(log(y) \sim x, data = train)
```



#### The Procedure

1. Log the outcome and fit a model

```
model <- Im(log(y) \sim x, data = train)
```

2. Make the predictions in log space

```
logpred <- predict(model, data = test)</pre>
```



#### The Procedure

1. Log the outcome and fit a model

```
model <- Im(log(y) \sim x, data = train)
```

2. Make the predictions in log space

```
logpred <- predict(model, data = test)</pre>
```

3. Transform the predictions to outcome space

```
pred <- exp(logpred)</pre>
```



# Predicting Log-transformed Outcomes: Multiplicative Error

$$log(a) + log(b) = log(ab)$$

$$log(a) - log(b) = log(a/b)$$

- Multiplicative error: pred/y
- Relative error:  $(pred y)/y = \frac{pred}{y} 1$

Reducing multiplicative error reduces relative error.



#### Root Mean Squared Relative Error

RMS-relative error = 
$$\sqrt{(\frac{pred-y}{y})^2}$$

- Predicting log-outcome reduces RMS-relative error
- But the model will often have larger RMSE



#### Example: Model Income Directly

```
modIncome <- Im(Income \sim AFQT + Educ, data = train)
```

- AFQT: Score on proficiency test 25 years before survey
- Educ: Years of education to time of survey
- Income: Income at time of survey



#### Model Performance

```
test %>%
mutate(pred = predict(modIncome, newdata = test),
err = pred - Income) %>%
summarize(rmse = sqrt(mean(err^2)),
rms.relerr = sqrt(mean( (err/Income)^2 )))
```

RMSE	RMS.relerr
36,819.39	3.295189



#### Model log(Income)

```
modLogIncome <- lm(log(Income) ~ AFQT + Educ, data = train)</pre>
```



#### Model Performance

RMSE	RMS.relerr
38,906.61	2.276865



### Compare Errors

log(Income) model: smaller RMS-relative error, larger RMSE

Model	RMSE	RMS-relative error
On Income	36,819.39	3.295189
On log(Income)	38,906.61	2.276865





SUPERVISED LEARNING IN R: REGRESSION

# Let's practice!





SUPERVISED LEARNING IN R: REGRESSION

# Transforming inputs before modeling

Nina Zumel and John Mount Win-Vector LLC



#### Why To Transform Input Variables

- Domain knowledge/synthetic variables
  - Intelligence  $\sim mass.brain/mass.body^{2/3}$



#### Why To Transform Input Variables

- Domain knowledge/synthetic variables
  - Intelligence  $\sim mass.brain/mass.body^{2/3}$
- Pragmatic reasons
  - Log transform to reduce dynamic range
  - Log transform because meaningful changes in variable are multiplicative

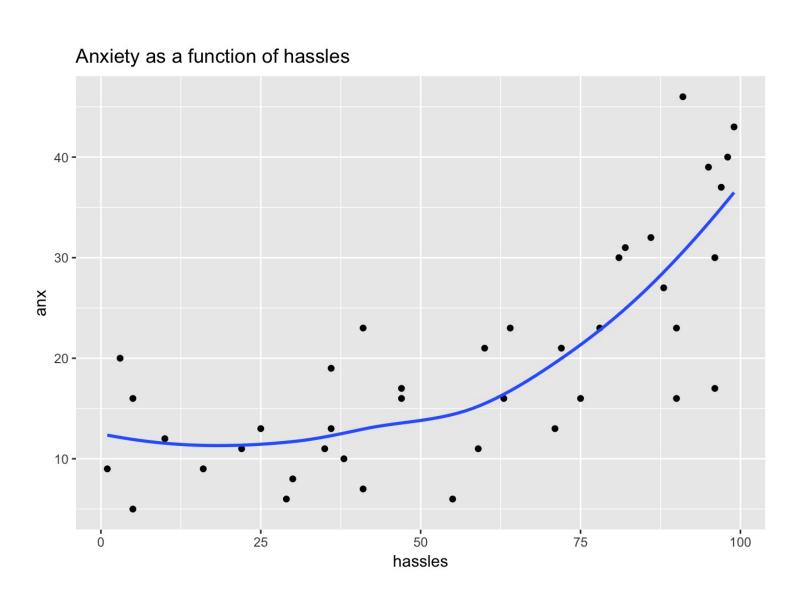


#### Why To Transform Input Variables

- Domain knowledge/synthetic variables
  - Intelligence  $\sim mass.brain/mass.body^{2/3}$
- Pragmatic reasons
  - Log transform to reduce dynamic range
  - Log transform because meaningful changes in variable are multiplicative
  - y approximately linear in f(x) rather than in x

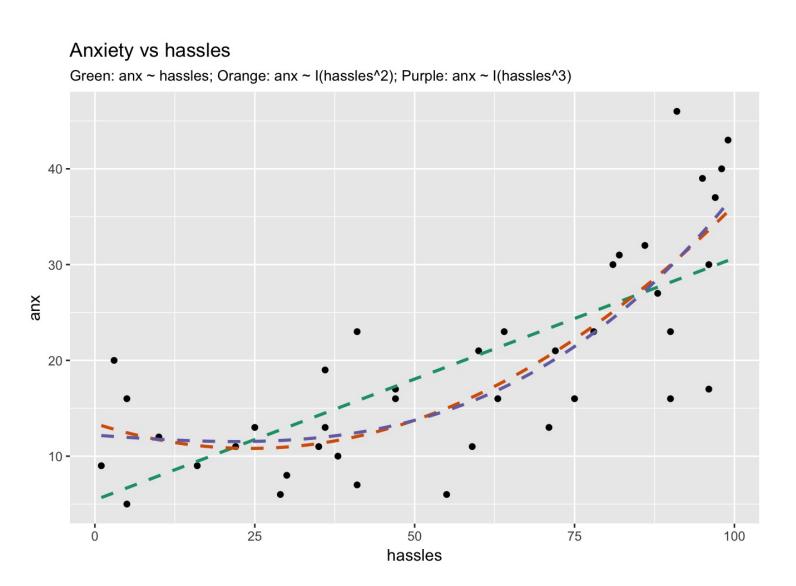


#### Example: Predicting Anxiety





#### Transforming the hassles variable





#### Different possible fits

#### Which is best?

- anx ~ I(hassles^2)
- anx ~ I(hassles^3)
- anx ~ I(hassles^2) + I(hassles^3)
- anx ~ exp(hassles)
- ...

I(): treat an expression literally (not as an interaction)



#### Compare different models

Linear, Quadratic, and Cubic models

```
mod_lin <- lm(anx ~ hassles, hassleframe)
summary(mod_lin)$r.squared

## [1] 0.5334847

mod_quad <- lm(anx ~ I(hassles^2), hassleframe)
summary(mod_quad)$r.squared

## [1] 0.6241029

mod_tritic <- lm(anx ~ I(hassles^3), hassleframe)
summary(mod_tritic)$r.squared

## [1] 0.6474421
```



#### Compare different models

Use cross-validation to evaluate the models

Model	RMSE
Linear (hassles)	7.69
Quadratic ( $hassles^2$ )	6.89
Cubic ( $hassles^3$ )	6.70





SUPERVISED LEARNING IN R: REGRESSION

# Let's practice!