Feature Engineering

Applied Machine Learning in R
Pittsburgh Summer Methodology Series

Lecture 2-A July 20, 2021

Overview

Feature Engineering

Prepare the predictors for analysis

- *Extract* predictors
- *Transform* predictors
- *Re-encode* predictors
- *Combine* predictors
- *Reduce* predictor dimensionality
- *Impute* missing predictor values
- *Select* and drop predictors

Motivation

Features are descriptions of the data points that help to predict the outcomes

- We may need to extract features from "raw" or "low-level" data (e.g., images)
- We may need to address issues with missing data and feature distributions

There are many potential ways to **encode** or "represent" the features/predictors

- e.g., adding, dropping, transforming, and combining predictors[1]
- predictor encoding can have a big **impact on predictive performance**[2]
- The optimal encoding depends on both the **algorithm** and the **relationships**

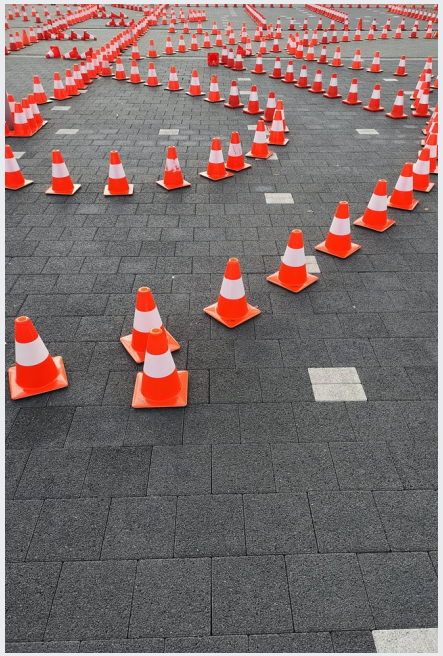
[1] Some algorithms can learn their own, complex feature representations
[2] Some algorithms are more sensitive to feature encoding than others

Examples of Feature Encodings

When an event or observation occurred

- The numeric year *(2021)*
- The numeric month *(7)*
- The numeric day of the month *(20)*
- The numeric day of the year *(201)*
- Days since a reference *(diagnosis +2)*
- The day of the week *(Tuesday)*
- The season of the year *(Summer)*
- The type of day *(weekday)*
- The presence of a holiday *(FALSE)*

Issues to Navigate in Feature Engineering



- predictors with **non-normal** distributions
- predictors with vastly **different scales**
- predictors with extreme **outliers**
- predictors with **missing** or censored values
- predictors that are **correlated** with one another
- predictors that are **redundant** with one another
- predictors that have zero or **near-zero variance**
- predictors that are **uninformative** for a task
- predictors with **uncertainty** or unreliability

Recipes for Feature Engineering

All of the predictor engineering steps can be done "by hand" in R

The {caret} package provides some basic convenience tools

We will be learning the {recipes} package from {tidymodels}

1. Initiate a recipe by declaring data and roles using `recipe()`
2. Add one or more preprocessing steps using `step_*()`
3. Prepare/estimate the preprocessing steps using `prep()`
4. Apply these steps to the training and testing data with `bake()`

Example Dataset: `titanic`

Rows: 963 passengers **Columns:** 7 variables

Variable	Description
survived	Did passenger survive? {FALSE, TRUE}
pclass	Passenger class {1st, 2nd, 3rd}
sex	Passenger sex {female, male}
age	Passenger age (years)
sibsp	Siblings and spouses Aboard (#)
parch	Parents and children Aboard (#)
fare	Cost of passenger fare ($)

Download the dataset from: https://osf.io/vmu93/

```r
# Import the dataset from file
library(tidyverse)
titanic <- read_csv("titanic.csv")

# Split the data
library(caret)
index <- createDataPartition(
  y = titanic$survived,
  p = 0.8,
  list = FALSE
)
titanic_train <- titanic[index, ]
titanic_test <- titanic[-index, ]
```

Recipes for Feature Engineering

```r
# There are three equivalent ways to specify variables and roles
library(recipes)

titanic_recipe <- recipe(
  titanic,
  vars = c("survived", "pclass", "sex", "age", "sibsp", "parch", "fare"),
  roles = c("outcome", "predictor", "predictor", "predictor",
            "predictor", "predictor", "predictor")
)

titanic_recipe <-
  recipe(titanic) %>%
  update_role(survived, new_role = "outcome")

titanic_recipe <- recipe(titanic, formula = survived ~ .)
```

Recipes for Feature Engineering

```
# Use summary() on a recipe to view a table of variables
titanic_recipe %>% summary()
```

variable	type	role	source
pclass	nominal	predictor	original
sex	nominal	predictor	original
age	numeric	predictor	original
sibsp	numeric	predictor	original
parch	numeric	predictor	original
fare	numeric	predictor	original
survived	nominal	outcome	original

Now we are ready to add some preprocessing (i.e., feature engineering) steps to the recipe!

Common Steps (Lecture Roadmap)

- **Adding predictors**
  - Calculated predictors
  - Categorical predictors
  - Interaction Terms
- **Transforming predictors**
  - Centering and Scaling
  - Addressing Non-normality
  - Adding Non-linearity
- **Reducing predictors**
  - Nero-Zero Variance
  - Multicollinearity
  - Dimensionality Reduction
- **Advanced Steps**
  - Feature Extraction
  - Dealing with Missing Values
  - Feature Selection

Adding predictors

Calculated predictors

Some variables will need to be calculated from existing values and variables

- You may choose to score an instrument from item-level data
- You may choose to encode a predictor as the ratio of two values
- You may choose to calculate sums, means, counts, proportions, etc.

We will show you some basic steps for calculating variables within {recipes}

For more advanced/complex data wrangling, we recommend you read

- *R for Data Science: Visualize, Model, Transform, Tidy, and Import Data* by Wickham and Grolemund (book for purchase or online for free)

Calculated predictors

```
# Add a step to calculate new predictors from existing predictors
cp_recipe <-
  titanic %>%
  recipe(survived ~ .) %>%
  step_mutate(
    numfamily = sibsp + parch,
    over70 = age > 70
  ) %>%
  prep(training = titanic_train, log_changes = TRUE)
#> step_mutate (mutate_ckkzk):
#>  new (2): numfamily, over70
```

Calculated predictors

```
cp_recipe %>% summary()
```

variable	type	role	source
pclass	nominal	predictor	original
sex	nominal	predictor	original
age	numeric	predictor	original
sibsp	numeric	predictor	original
parch	numeric	predictor	original
fare	numeric	predictor	original
survived	nominal	outcome	original
numfamily	numeric	predictor	derived
over70	logical	predictor	derived

Calculated predictors

```
# bake() will allow us to generate updated training and testing sets
cp_train <- bake(cp_recipe, new_data = titanic_train)
cp_test <- bake(cp_recipe, new_data = titanic_test)
```

```
cp_test
```

pclass	sex	age	sibsp	parch	fare	survived	numfamily	over70
1st	female	25.0000	1	2	151.5500	no	3	FALSE
1st	male	80.0000	0	0	30.0000	yes	0	TRUE
1st	male	45.0000	0	0	35.5000	no	0	FALSE
1st	female	30.0000	0	0	164.8667	yes	0	FALSE
1st	male	42.0000	0	0	26.5500	no	0	FALSE

Categorical predictors

Categorical predictors can be re-encoded into multiple binary (0 or 1) predictors

In `titanic`, the categorical variable `sex` takes on the value *male* or *female*

One-Hot Encoding

sex	sex_female	sex_male
female	1	0
male	0	1

Simple and easy to interpret
Good for tree-based methods

Dummy Coding

sex	sex_male
female	0
male	1

Efficient and avoids redundancy
Good for GLM-based methods

Categorical predictors in R

```
# Add a step to add one hot encoding
oh_recipe <-
  titanic %>%
  recipe(survived ~ .) %>%
  step_dummy(pclass, sex, one_hot = TRUE) %>%
  prep(training = titanic_train, log_changes = TRUE)
#> step_dummy (dummy_m0AXx):
#>  new (5): pclass_X1st, pclass_X2nd, pclass_X3rd, sex_female, sex_male
#>  removed (2): pclass, sex
```

[1] As a shortcut, we could also have used `all_nominal_predictors()` instead of `pclass, sex`.

Categorical predictors in R

```
# Add a step to the recipe to create dummy codes for pclass and sex
dc_recipe <-
  titanic %>%
  recipe(survived ~ .) %>%
  step_dummy(pclass, sex, one_hot = FALSE) %>%
  prep(training = titanic_train, log_changes = TRUE)
#> step_dummy (dummy_q60jm):
#>  new (3): pclass_X2nd, pclass_X3rd, sex_male
#>  removed (2): pclass, sex
```

[1] As another shortcut, I could leave off `one_hot = FALSE` since that is the default option.

Interaction Terms

Interaction terms allow the meaning of one predictor to depend on other predictors

In this way, interaction terms allow predictor "effects" to be **contingent** or **conditional**

e.g., perhaps having parents or children on board the Titanic helps you predict survival... but the effects differs depending on whether the passenger is a man or a woman

Interaction terms are literally **products** (i.e., multiplications) of two or more predictors

In order to include categorical variables in interaction terms, dummy code them first

Interaction Terms in R

```
# Add interaction terms using formula notation
it_recipe <-
  titanic %>%
  recipe(survived ~ .) %>%
  step_dummy(pclass, sex) %>%
  step_interact(~ age:parch + sibsp:starts_with("pclass_")) %>%
  prep(training = titanic_train, log_changes = TRUE)
#> step_dummy (dummy_Y487O):
#>  new (3): pclass_X2nd, pclass_X3rd, sex_male
#>  removed (2): pclass, sex
#>
#> step_interact (interact_IuhSn):
#>  new (3): age_x_parch, sibsp_x_pclass_X2nd, sibsp_x_pclass_X3rd
```

[1] The selector function `starts_with()` allows you to easily capture all dummy codes for a variable.

Interaction Terms in R

```
# Bake the recipe and preview the updated training set
it_train_baked <- bake(it_recipe, new_data = titanic_train)
```

age	sibsp	parch	fare	survived	pclass_X2nd	pclass_X3rd	sex_male	age_x_parch	sibsp_x_pclass_
29.0000	0	0	211.3375	yes	0	0	0	0.0000	
0.9167	1	2	151.5500	yes	0	0	1	1.8334	
30.0000	1	2	151.5500	no	0	0	1	60.0000	
48.0000	0	0	26.5500	yes	0	0	1	0.0000	
63.0000	1	0	77.9583	yes	0	0	0	0.0000	
53.0000	2	0	51.4792	yes	0	0	0	0.0000	

Comprehension Check #1

Question 1

What is the correct order in which to add the {recipe} functions to a pipeline?

a) recipe > prep > step(s) > bake

b) recipe > step(s) > prep > bake

c) prep > step > bake > recipe

d) prep > recipe > step > bake

Question 2

How many dummy codes are needed to encode a variable with five (5) categorical levels?

a) Six (6)

b) Five (5)

c) Four (4)

d) One (1)

Transforming predictors

Normalizing

Predictors with vastly different means and SDs can cause problems for some algorithms

Centering a predictor involves changing its mean to 0.0

- This is accomplished by subtracting the mean from every observation

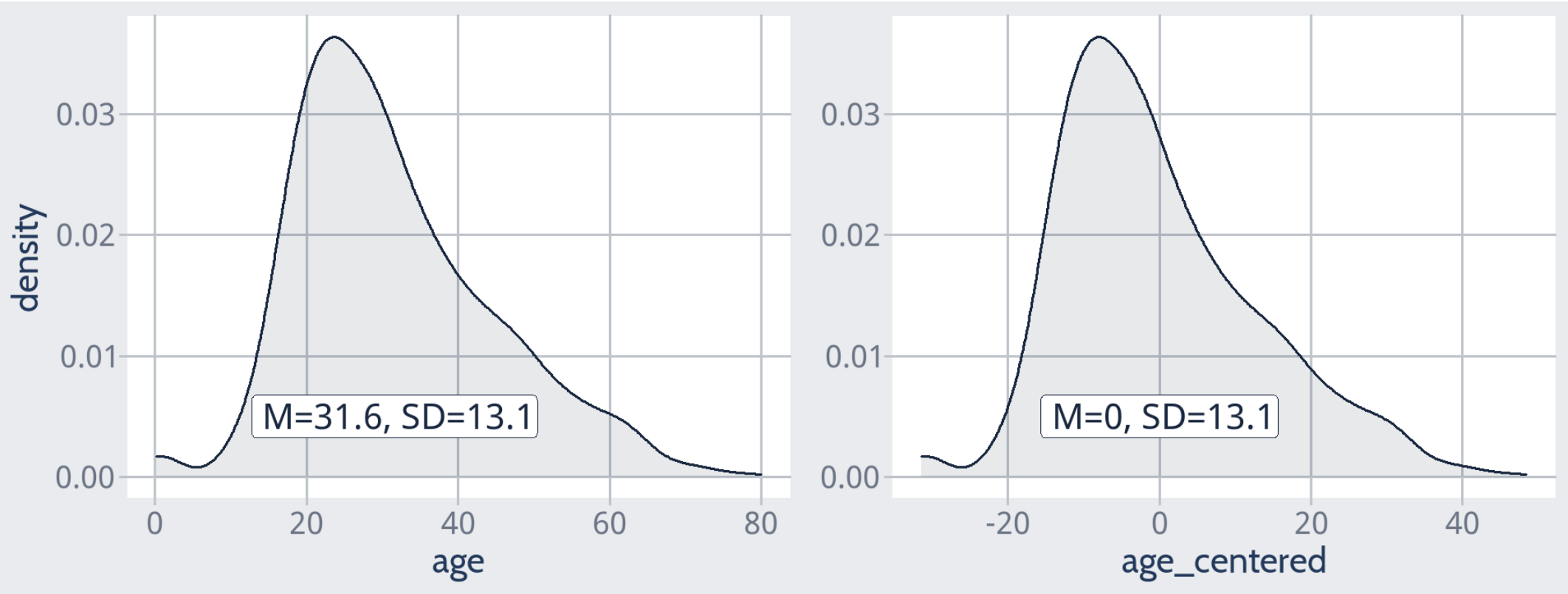
Scaling a predictor involves changing its standard deviation (and variance) to 1.0

- This is accomplished by dividing each observation by the standard deviation

Normalizing a predictor involves centering it and then scaling it

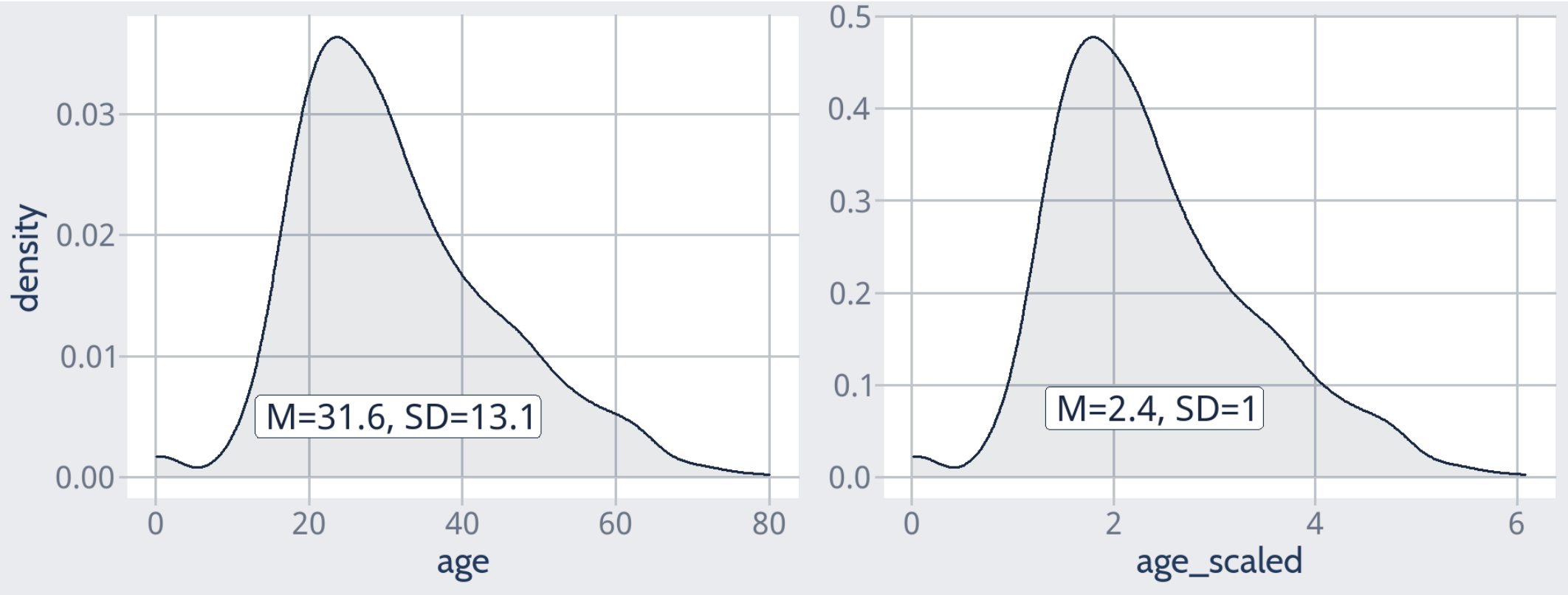
- This is also sometimes called "standardizing" or z-scoring the predictor

Centering Visualized



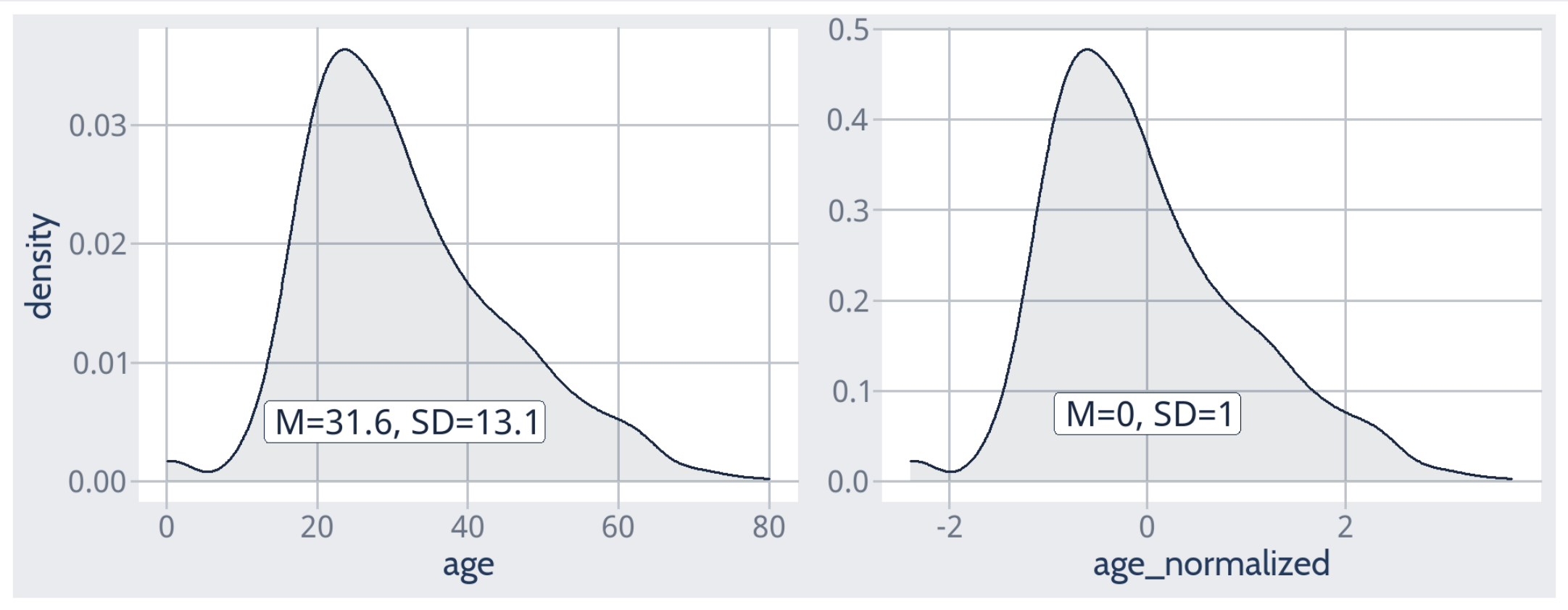
The mean is now 0 but the shape and SD of the distribution are unchanged (i.e., it has been shifted left).

Scaling Visualized



The SD is now 1 and the mean is lower, but the shape of the distribution is unchanged.

Normalizing Visualized



The mean is now 0 and the SD is now 1, but the shape of the distribution is unchanged.

Normalizing in R

```
# Normalize the age variable using the training set mean and SD
norm_recipe <-
  titanic %>%
  recipe(survived ~ .) %>%
  step_normalize(age) %>%
  prep(training = titanic_train, log_changes = TRUE)
#> step_normalize (normalize_nKovC): same number of columns
```

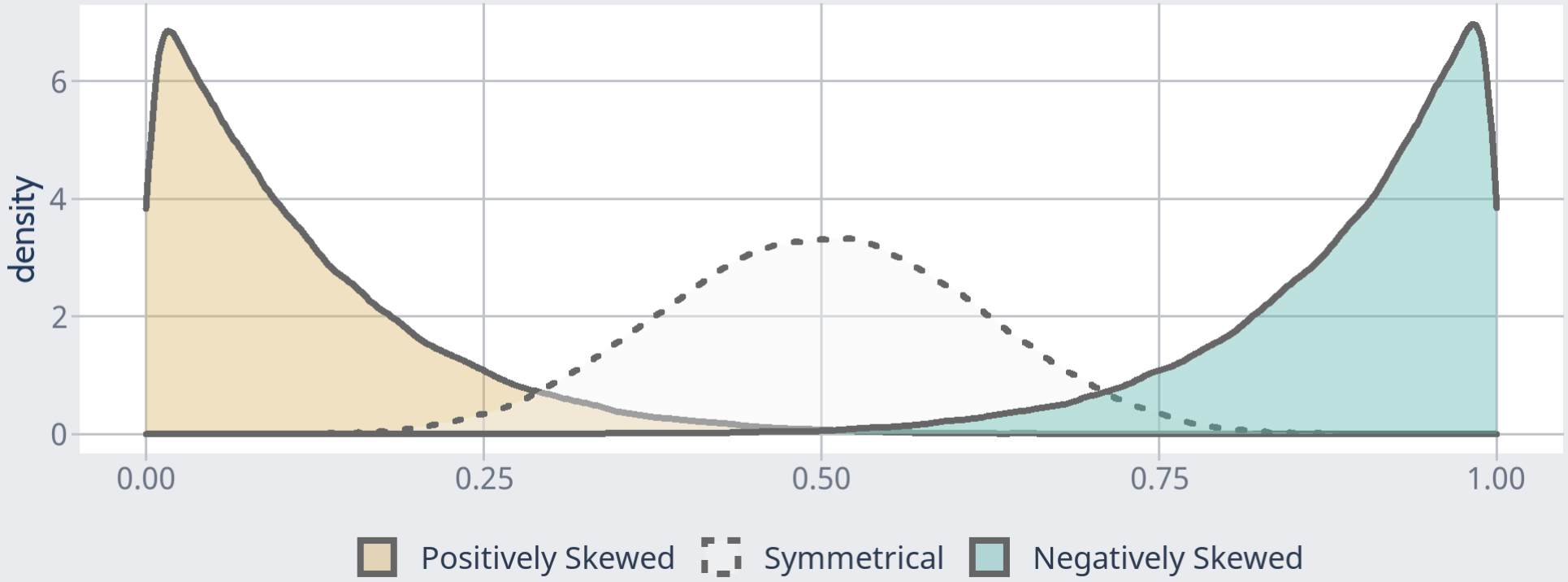
```
# Because of prep(), bake() uses the training set mean and SD[2]
norm_test <- bake(norm_recipe, new_data = titanic_test)
```

[1] We could also have used `step_center()` and/or `step_scale()` instead of `step_normalize()`.
[2] This is important to accurately estimating out-of-sample performance on truly novel data.

Addressing Non-normality

A **skewed** distribution is one that is not symmetric (i.e., it has a "heavy tail")

A **bounded** distribution is one that cannot go beyond certain boundary values



Addressing Non-normality

Specific transformations (e.g., log, inverse, logit) can help address specific issues

The Box-Cox and Yeo-Johnson approaches employ **families of transformations**

Box-Cox cannot be applied to negative or zero values, but **Yeo-Johnson** can

$$x^{\star}_{(yj)} = \begin{cases} ((x+1)^{\lambda} - 1)/\lambda & \text{if } \lambda \neq 0, x \geq 0 \\ \log(x+1) & \text{if } \lambda = 0, x \geq 0 \\ -[(-x+1)^{2-\lambda} - 1)]/(2-\lambda) & \text{if } \lambda \neq 2, x < 0 \\ -\log(-x+1) & \text{if } \lambda = 2, x < 0 \end{cases}$$

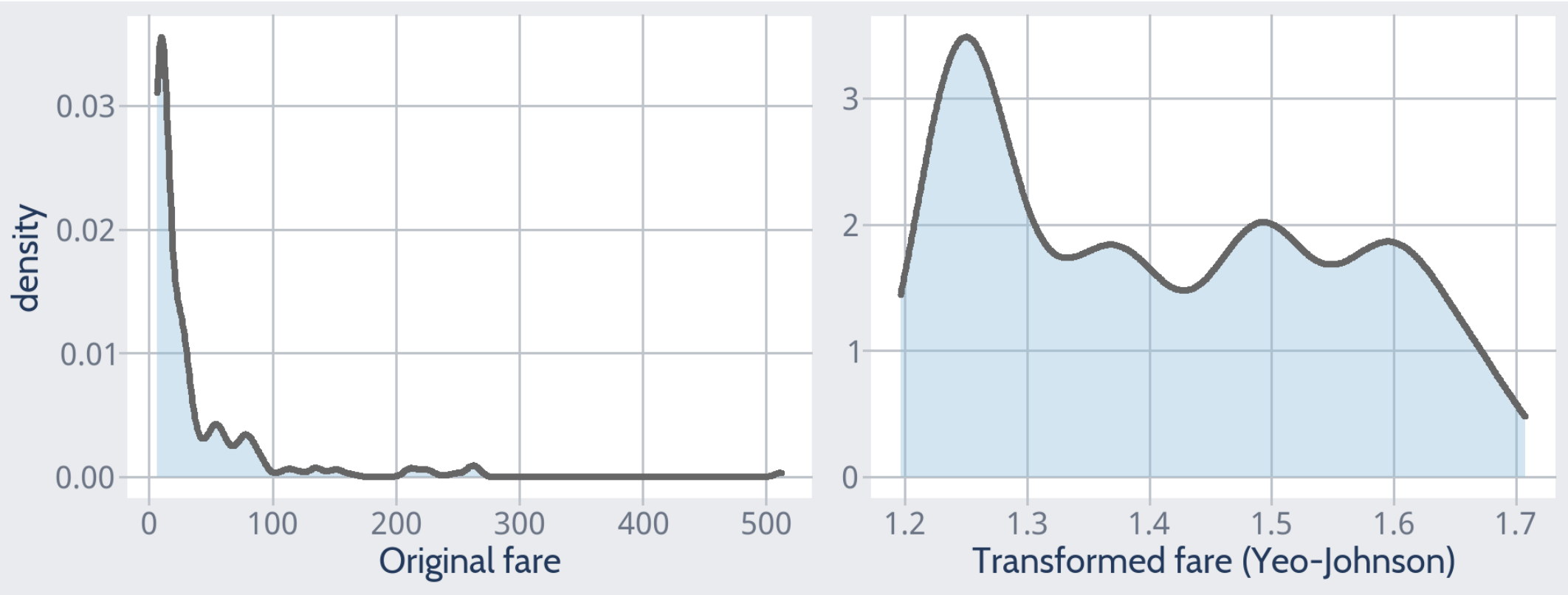
Addressing Non-normality in R

```
# Add step to apply the Yeo-Johnson transformation to fare
yj_recipe <-
  titanic %>%
  recipe(survived ~ .) %>%
  step_YeoJohnson(fare) %>%
  prep(training = titanic_train, log_changes = TRUE)
#> step_YeoJohnson (YeoJohnson_fotF2): same number of columns
```

[1] If you would like to use specific transformations, use: `step_log()`, `step_inverse()`, `step_sqrt()`, etc.
[2] As with normalizing, use `prep()` to estimate λ from training set and use it when you `bake()` the test set.

Addressing Non-normality in R

Bake the recipe using the training data and then plot the transformed variable



Adding Nonlinearity

Many relationships between features and labels are non-linear in nature

- *e.g., perhaps survival was lowest for young adults and higher for children and elders*

Successful prediction will require us to **model that nonlinearity** in such cases

Many algorithms can capture nonlinearity easily but others need our help

- For these algorithms, we can provide help through feature engineering
- This typically means adding **nonlinear expansions** of existing predictors[1]

[1] If you are familiar with polynomial (e.g., quadratic or cubic) regression, you already have relevant experience!

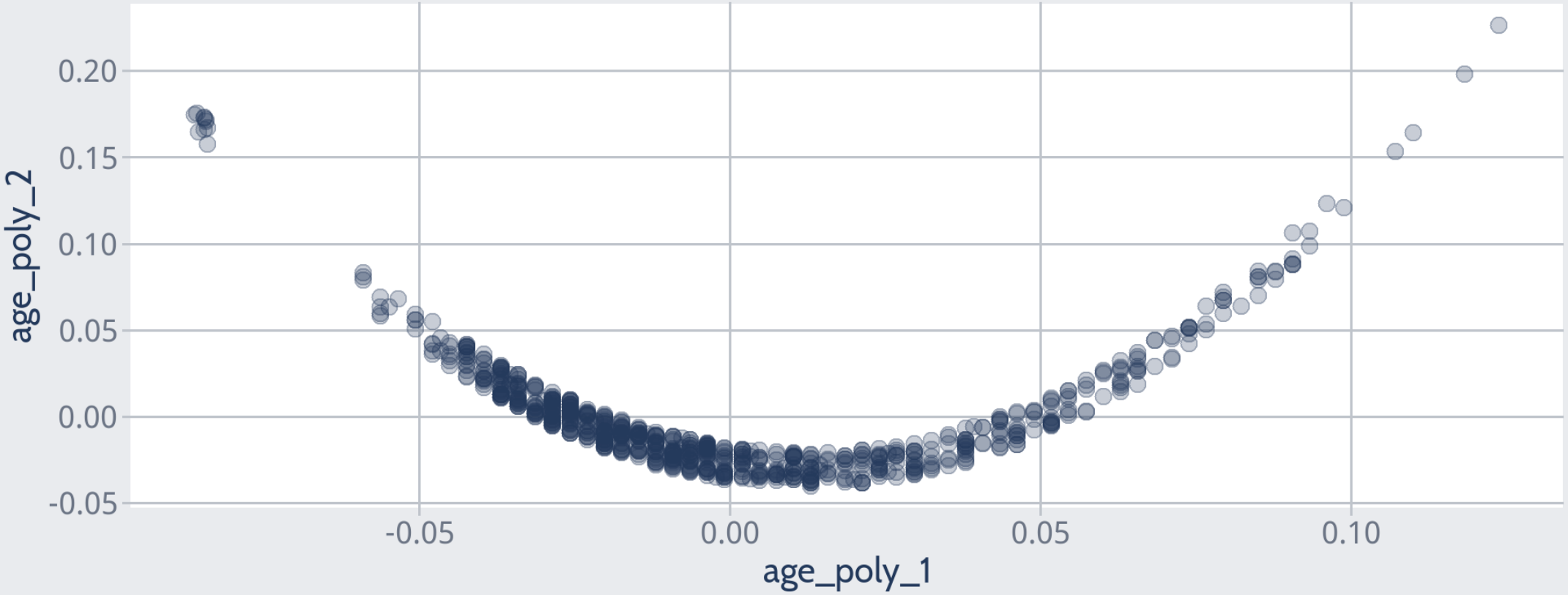
Adding Nonlinearity in R

```
# Add step to add orthogonal polynomial basis functions
nl_recipe <-
  titanic %>%
  recipe(survived ~ .) %>%
  step_poly(age, degree = 2) %>%
  prep(training = titanic_train, log_changes = TRUE)
#> step_poly (poly_gBTGQ):
#>  new (2): age_poly_1, age_poly_2
#>  removed (1): age
```

[1] Note that, by specifying `degree = 2`, we are creating a quadratic expansion; more flexibility can be added.
[2] Additional nonlinear expansions are also available: `step_ns()`, `step_bs()`, and `step_hyperbolic()`.

Adding Nonlinearity in R

Bake the recipe and plot the polynomial terms against one another (with vertical jitter).



Comprehension check #2

Question 1

I want to transform two predictors to have the same variance. Which would NOT achieve this?

a) Centering both

b) Scaling both

c) Normalizing both

d) Dividing each by its SD

Question 2

Which of the following issues would the Yeo-Johnson transformation NOT help with?

a) Positive skew

b) Negative skew

c) Outlier values

d) Categorical data

Reducing predictors

Zero and Near-Zero Variance Predictors

Zero variance predictors take on only a single value in the sample

- These predictors are **uninformative** and may lead to **modeling problems**

Near-zero variance predictors take on only a few unique values with low frequencies

- These predictors can easily become zero-variance predictors during resampling

For many algorithms, we want to **detect** and **remove** both types of predictors

(This may not be necessary for algorithms with built-in *predictor selection*)

Zero and Nero-Zero Variance Predictors in R

```
# Detect and remove zero-variance predictors
zv_recipe <-
  titanic %>%
  recipe(survived ~ .) %>%
  step_mutate(
    species = "homo sapiens", # will have zero variance
    over70 = age > 70 # will have near-zero variance
  ) %>%
  step_zv(all_predictors()) %>%
  prep(training = titanic_train, log_changes = TRUE)
#> step_mutate (mutate_DcJWI):
#>  new (2): species, over70
#>
#> step_zv (zv_J6XEM):
#>  removed (1): species
```

Zero and Nero-Zero Variance Predictors in R

```
# Detect and remove near-zero-variance predictors
nzv_recipe <-
  titanic %>%
  recipe(survived ~ .) %>%
  step_mutate(
    species = "homo sapiens",  # will have zero variance
    over70 = age > 70 # will have near-zero variance
  ) %>%
  step_nzv(all_predictors()) %>%
  prep(training = titanic_train, log_changes = TRUE)
#> step_mutate (mutate_oFb8f):
#>  new (2): species, over70
#>
#> step_nzv (nzv_pBfm2):
#>  removed (2): species, over70
```

Multicollinearity

Highly correlated predictors can lead to problems for some algorithms/procedures

- The model has to randomly choose between the predictors, leading to **instability**
- Model predictions may be fine, but model **interpretation** will often be obfuscated
- The cutoff for "problematically high" correlations varies (e.g., 0.5 to 0.9 or higher)

Predictors that are **linear combinations** of other predictors are similarly problematic

- Occurs if a predictor variable can be predicted from the other predictor variables
- This is why dummy coding is preferred to one-hot encoding for some algorithms

For many algorithms, we want to **detect** and **remove** redundant predictors

(This may not be necessary for algorithms with *regularization* or *predictor selection*)

Multicollinearity in R

```
# Add some predictors with high correlations and linear dependency
mc_titanic <- titanic %>% mutate(
  wisdom = 100 + 0.25 * age + rnorm(nrow(.)), # high corr
  numfamily = sibsp + parch # linear combination
)
mc_train <- mc_titanic[index, ]
```

Multicollinearity in R

```
library(correlation)
correlation(mc_train) %>% filter(abs(r) > 0.75)
```

Table: Correlation Matrix (pearson-method)

Parameter1	Parameter2	r	95% CI	t(770)	p
age	wisdom	0.95	(0.95, 0.96)	88.62	< .001*
sibsp	numfamily	0.81	(0.78, 0.83)	38.28	< .001*
parch	numfamily	0.81	(0.79, 0.84)	38.80	< .001*

p-value adjustment method: Holm (1979) Observations: 772

Multicollinearity in R

```
# Detect and remove predictors that are highly correlated
hc_recipe <-
  mc_titanic %>%
  recipe(survived ~ .) %>%
  step_corr(all_numeric_predictors(), threshold = 0.9) %>%
  prep(training = mc_train, log_changes = TRUE)
#> step_corr (corr_TtuNr):
#>  removed (1): age
```

[1] If we want to consider correlations with categorical variables, we can add `step_dummy()` to the pipeline.
[2] We could have also lowered the threshold to 0.8 in order to drop the `family` variable here.

Multicollinearity in R

```
# Detect and remove predictors that are linear combinations
lc_recipe <-
  mc_titanic %>%
  recipe(survived ~ .) %>%
  step_lincomb(all_numeric_predictors()) %>%
  prep(training = mc_train, log_changes = TRUE)
#> step_lincomb (lincomb_jEsnD):
#>  removed (1): numfamily
```

Dimensionality Reduction

Each feature/predictor included can be considered an additional "dimension"

Dimensionality reduction techniques try to find a smaller set of predictors to use

- If successful, little information from the original set of predictors will be lost
- Most techniques create new predictors as *functions of the original predictors*

Principal Components Analysis (PCA) is a commonly used technique

- The new predictors (PCs) are *linear combinations* of the original predictors
- The PCs are *uncorrelated* with one another, thus addressing multicollinearity
- PCs are extracted until a target amount of variability is explained (e.g., 75%)

[1] Predictors should be normalized (i.e., centered and scaled) before PCA is used.
[2] PCA is linear and unsupervised but there are nonlinear and supervised techniques.

Dimensionality Reduction in R

```
# Normalize numeric predictors and then do PCA
pca_recipe <-
  titanic %>%
  recipe(survived ~ .) %>%
  step_normalize(all_numeric_predictors()) %>%
  step_pca(all_numeric_predictors(), threshold = 0.75) %>%
  prep(training = titanic_train, log_changes = TRUE)
#> step_normalize (normalize_tI1if): same number of columns
#>
#> step_pca (pca_bOpoZ):
#>  new (3): PC1, PC2, PC3
#>  removed (4): age, sibsp, parch, fare
```

[1] Note that PCA is most effective when there are many correlated predictors, so this is a weak use of it.

Advanced Topics

Feature Extraction

Feature extraction involves generating features from "raw" data

For raw **text** data, natural language processing techniques can be used

- *e.g., sentiment, word frequencies, word relationships, topic modeling, syntax*

For raw **image** and video data, computer vision techniques can be used

- *e.g., edges, corners, blobs, ridges, objects, curvature, shape, motion, color*

For raw **audio** data, acoustic signal processing techniques can be used

- *e.g., rhythm, stress, intonation, pitch, loudness, glottal flow, spectral density*

[1] One of the strengths of deep learning is its ability to learn its own feature representations from raw data.

Dealing with Missing Values

There are several approaches to handling missing values in predictors

- Some algorithms (e.g., tree-based techniques) handle missing data inherently
- Another option is to drop predictors with any (or a lot of) missing values
- Or we can **impute** or estimate the missing values based on the other predictors

There are many techniques for imputing missing predictor values

- Some are very simple (e.g., using the mean or median) and others more complex
- We can also use a linear model or even machine learning to impute missing values
- {recipes} provides functions: `step_impute_mean()`, `step_impute_knn()`, etc.

[1] Missing data tends to be more problematic for inferential modeling than predictive modeling.
[2] When imputing, it is a good idea to use cross-validation to capture the uncertainty in the imputations.

Feature Selection

Feature selection is focused on removing uninformative or redundant predictors

- Models with fewer predictors may be more interpretable, accurate, and efficient

Wrapper methods compare models with different combinations of predictors

- These are algorithms that search for combinations that optimize performance
- These methods tend to perform well but can be computationally expensive

Filter methods evaluate predictors outside of the context of the predictive model[1]

- Only predictors that seem informative, relevant, or unique will be retained
- These methods don't perform as well but are computationally efficient

[1] Note that we have already learned some basic filter methods (e.g., `step_corr()` and `step_nzv()`).

Live Coding Activity

Live Coding Activity

I will show you a new dataset and the process of feature engineering in RStudio

- If you have one small screen, I recommend you just watch the process
- With a large screen or multiple screens, you can follow along in RStudio

Afterward, there will be a hands-on activity where you will modify my code

If you have questions, please post them in chat or in the workshop Slack channel

[1] All files can be accessed from the workshop website: https://osf.io/3qhc8/

Hands-on Activity

Modify the Live Coding example code to accomplish the following goals:

1. Use 75% of the data for training and 25% of the data for testing.
2. Apply the Yeo-Johnson transformation to `flight_distance` (before normalizing)
3. Instead of using PCA to address multicollinearity, drop highly correlated predictors.
4. Use one-hot encoding for the nominal predictors instead of dummy codes.
5. Add an interaction term that conditions `seat_comfort` on `flight_distance`

BONUS: Read the Recommended preprocessing appendix from the TMWR book

FURTHER READING: TMWR Recipes Chapter, Feature Engineering and Selection Book

Time for a Break!

10:00