Median imputation

MACHINE LEARNING TOOLBOX

Max Kuhn

Software Engineer at RStudio and creator of caret

Dealing with missing values

- Most models require numbers, can't handle missing data
- Common approach: remove rows with missing data
    - Can lead to biases in data
    - Generate over-confident models
- Better strategy: median imputation!
    - Replace missing values with medians
    - Works well if data missing at random (MAR)

Example: mtcars

```r
# Generate some data with missing values
data(mtcars)
set.seed(42)
mtcars[sample(1:nrow(mtcars), 10), "hp"] <- NA
```

```r
# Split target from predictors
Y <- mtcars$mpg
X <- mtcars[, 2:4]
```

```r
# Try to fit a caret model
library(caret)
model <- train(X, Y)
```

```
Error in train.default(X, Y) : Stopping
```

A simple solution

```r
# Now fit with median imputation
model <- train(X, Y, preProcess = "medianImpute")
print(model)
```

```
Random Forest

32 samples
 3 predictor

Pre-processing: median imputation (3)
Resampling: Bootstrapped (25 reps)
Summary of sample sizes: 32, 32, 32, 32, 32, 32, ...
Resampling results across tuning parameters:

  mtry  RMSE      Rsquared
  2     2.617096  0.8234652
  3     2.670550  0.8164535

RMSE was used to select the optimal model using the smallest value.
The final value used for the model was mtry = 2.
```

Let’s practice!

MACHINE LEARNING TOOLBOX

KNN imputation

MACHINE LEARNING TOOLBOX

Zach Mayer

Data Scientist at DataRobot and co-author of caret

Dealing with missing values

- Median imputation is fast, but…
- Can produce incorrect results if data missing not at random
- k-nearest neighbors (KNN) imputation
- Imputes based on "similar" non-missing rows

Example: missing not at random

- Pretend smaller cars don't report horsepower
- Median imputation incorrect in this case: it assumes small cars have medium-large horsepower

```r
# Generate data with missing values
mtcars[mtcars$disp < 140, "hp"] <- NA
Y <- mtcars$mpg
X <- mtcars[, 2:4]

# Use median imputation
model <- train(X, Y, method = "glm", preProcess = "medianImpute")
print(min(model$results$RMSE))
```

```
3.612713
```

Example: missing not at random

- KNN imputation is better
- Uses cars with similar disp / cyl to impute
- Yields a more accurate (but slower) model

```r
# Use KNN imputation
set.seed(42)
model <- train(
  X, Y, method = "glm", preProcess = "knnImpute"
)
print(min(model$results$RMSE))
```

```
3.558881
```

Let’s practice!

MACHINE LEARNING TOOLBOX

Multiple preprocessing methods

MACHINE LEARNING TOOLBOX

Zach Mayer
Data Scientist at DataRobot and co-author of caret

The wide world of preProcess

- You can do a lot more than median or knn imputation!
- Can chain together multiple preprocessing steps
- Common "recipe" for linear models (order matters!)
    - Median imputation $\Rightarrow$ center $\Rightarrow$ scale $\Rightarrow$ fit glm
- See `?preProcess` for more detail

Example: preprocessing mtcars

```r
# Generate some data with missing values
data(mtcars)
set.seed(42)
mtcars[sample(1:nrow(mtcars), 10), "hp"] <- NA
Y <- mtcars$mpg
X <- mtcars[,2:4] # <- Missing at random
```

```r
# Use linear model "recipe"
set.seed(42)
model <- train(
  X, Y, method = "glm",
  preProcess = c("medianImpute", "center", "scale")
)
print(min(model$results$RMSE))
```

```
3.612713
```

Example: preprocessing mtcars

```
# PCA before modeling
set.seed(42)
model <- train(
  X, Y, method = "glm",
  preProcess = c("medianImpute", "center", "scale", "pca")
)
min(model$results$RMSE)
```

```
3.402557
```

Example: preprocessing mtcars

```
# Spatial sign transform
set.seed(42)
model <- train(
  X, Y, method = "glm",
  preProcess = c("medianImpute", "center", "scale", "spatialSign")
)
min(model$results$RMSE)
```

```
4.284904
```

Preprocessing cheat sheet

- Start with median imputation
- Try KNN imputation if data missing not at random
- For linear models ...
  - Center and scale
  - Try PCA and spatial sign
- Tree-based models don't need much preprocessing

Let’s practice!

MACHINE LEARNING TOOLBOX

Handling low-information predictors

MACHINE LEARNING TOOLBOX

Zach Mayer
Data Scientist at DataRobot and co-author of caret

No (or low) variance variables

- Some variables don't contain much information
  - Constant (i.e. no variance)
  - Nearly constant (i.e. low variance)
- Easy for one fold of CV to end up with constant column
  - Can cause problems for your models
- Usually remove extremely low variance variables

Example: constant column in mtcars

```r
# Reproduce dataset from last video
data(mtcars)
set.seed(42)
mtcars[sample(1:nrow(mtcars), 10), "hp"] <- NA
Y <- mtcars$mpg
X <- mtcars[, 2:4]
```

```r
# Add constant-valued column to mtcars
X$bad <- 1
```

Example: constant column in mtcars

```r
# Try to fit a model with PCA + glm
model <- train(
  X, Y, method = "glm",
  preProcess = c("medianImpute", "center", "scale", "pca") )
```

```
Warning in preProcess.default(thresh = 0.95, k = 5, method = c("medianImpute",   :
  These variables have zero variances: bad
Something is wrong; all the RMSE metric values are missing:
      RMSE        Rsquared
 Min.   : NA   Min.   : NA
 1st Qu.: NA   1st Qu.: NA
 Median : NA   Median : NA
 Mean   :NaN   Mean   :NaN
 3rd Qu.: NA   3rd Qu.: NA
 Max.   : NA   Max.   : NA
 NA's   :1     NA's   :1
```

caret to the rescue (again)

- "zv" removes constant columns
- "nzv" removes nearly constant columns

```r
# Have caret remove those columns during modeling
set.seed(42)
model <- train(
  X, Y, method = "glm",
  preProcess = c("zv", "medianImpute", "center", "scale", "pca")
)
min(model$results$RMSE)
```

```
3.402557
```

Let’s practice!

MACHINE LEARNING TOOLBOX

Principle components analysis (PCA)

MACHINE LEARNING TOOLBOX

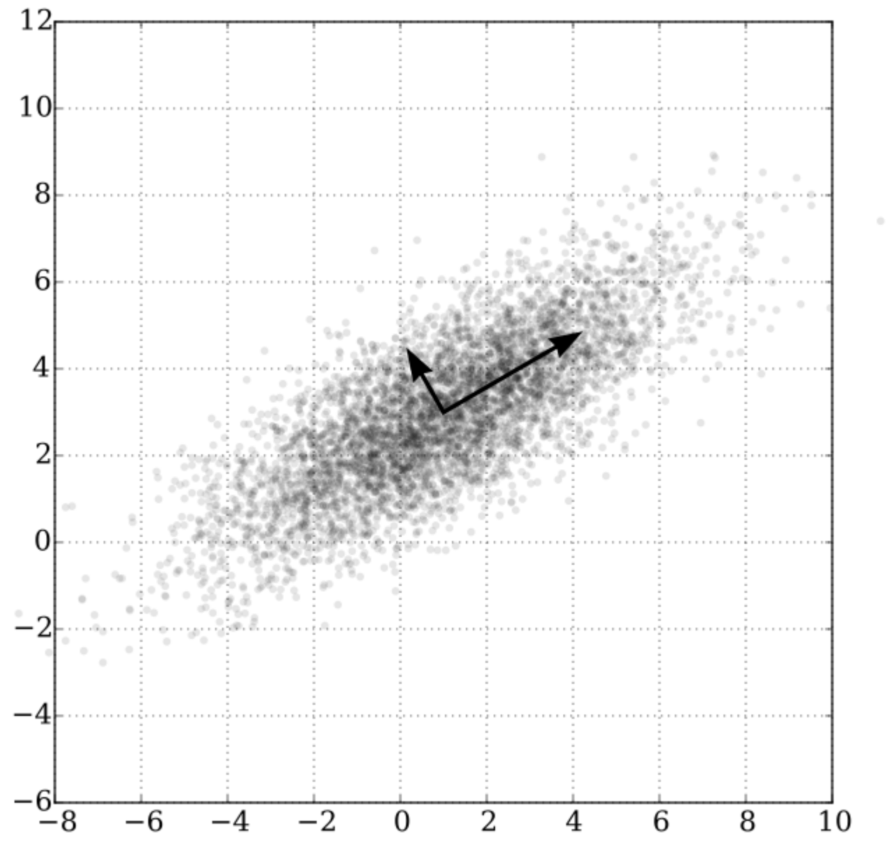
Zach Mayer
Data Scientist at DataRobot and co-author of caret

Principle components analysis

- Combines low-variance and correlated variables
- Single set of high-variance, perpendicular predictors
- Prevents collinearity (i.e. correlation among predictors)

PCA: a visual representation

- First component has highest variance
- Second component has second highest variance
- And so on ...



Example: blood-brain data

- Lots of predictors
- Many of them low-variance

```r
# Load the blood brain dataset
data(BloodBrain)
names(bbbDescr)[nearZeroVar(bbbDescr)]
```

```
[1] "negative"     "peoe_vsa.2.1" "peoe_vsa.3.1"
[4] "a_acid"       "vsa_acid"     "frac.anion7."
[7] "alert"
```

Example: blood-brain data

```r
# Basic model
set.seed(42)
data(BloodBrain)
model <- train(
  bbbDescr,
  logBBB,
  method = "glm",
  trControl = trainControl(
    method = "cv", number = 10, verbose = TRUE
  ),
  preProcess = c("zv", "center", "scale")
)
min(model$results$RMSE)
```

```
1.107702
```

Example: blood-brain data

```r
# Remove low-variance predictors
set.seed(42)
data(BloodBrain)
model <- train(
  bbbDescr,
  logBBB,
  method = "glm",
  trControl = trainControl(
    method = "cv", number = 10, verbose = TRUE
  ),
  preProcess = c("nzv", "center", "scale")
)
min(model$results$RMSE)
```

```
0.9796199
```

Example: blood-brain data

```r
# Add PCA
set.seed(42)
data(BloodBrain)
model <- train(
  bbbDescr,
  logBBB,
  method = "glm",
  trControl = trainControl(
    method = "cv", number = 10, verbose = TRUE
  ),
  preProcess = c("zv", "center", "scale", "pca")
)
min(model$results$RMSE)
```

```
0.9796199
```

Let’s practice!

MACHINE LEARNING TOOLBOX