

Median imputation

MACHINE LEARNING WITH CARET IN R



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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

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

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

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

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

A simple solution

```
# 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!

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KNN imputation

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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

```
# 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

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

```
3.558881
```

Let's practice!

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Multiple preprocessing methods

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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

```
# 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
```

```
# 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!

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Handling low-information predictors

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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

```
# 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]
```

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

Example: constant column in mtcars

```
# 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

```
# 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!

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Principle components analysis (PCA)

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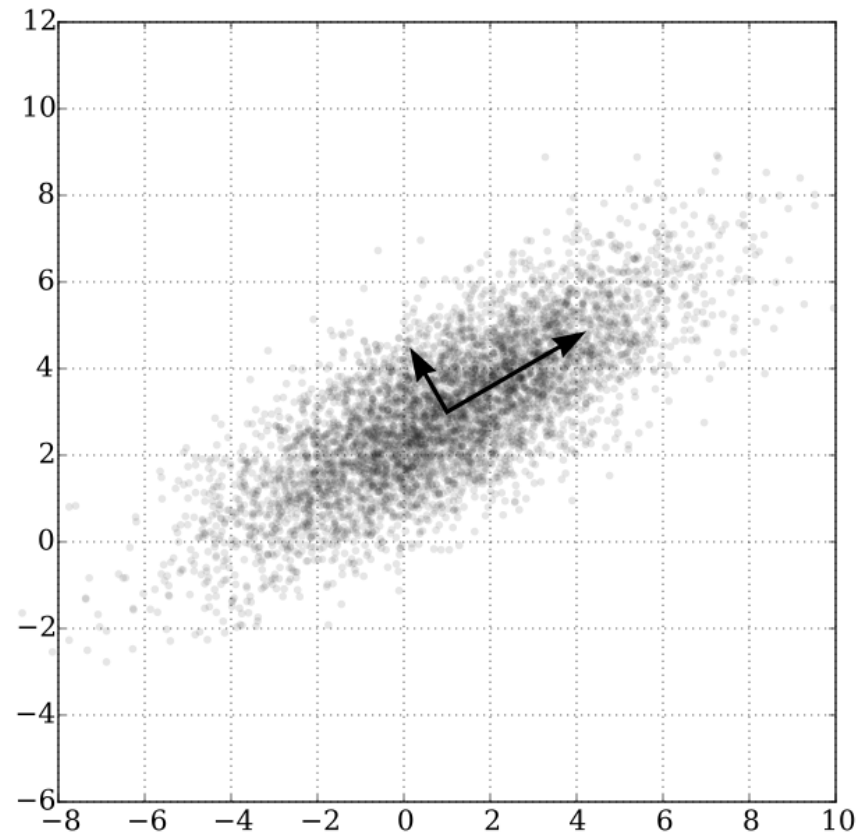
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Principle components analysis

- 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

```
# 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

```
# 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

```
# 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

```
# 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!

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