

Concepts in Machine Learning

Winter Institute in Data Science

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Building Models

Modeling Helper Functions

Example: `mtcars`

Example: Social Pressure Experiment (`recipes`)

Regularization Methods: LASSO, ridge regression, elastic nets

Building Models

How do we build models?

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What are our goals?

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1. Generative modeling
2. Predictive modeling

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2. Predictive modeling

Breiman (2001)

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- ▶ Theory
(novel theory, prior theory, prior findings)

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- ▶ Specification searching
(repeat modeling with same data)

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(novel theory, prior theory, prior findings)
- ▶ Raw data
(“data look nonlinear, so $\dots + \beta x^2 + \dots$ ”)
- ▶ Specification searching
(repeat modeling with same data)
- ▶ Training and testing
(repeat modeling, different data)

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- ▶ Confounders
- ▶ Pre-treatment only
- ▶ Avoid post-treatment
- ▶ “In-horizon”
- ▶ Test something “out-of-horizon”

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- ▶ Confounders
- ▶ Pre-treatment only
- ▶ Avoid post-treatment
- ▶ “In-horizon”
- ▶ Test something “out-of-horizon”

(Sometimes it will depend on goals.)

What to include, when thousands of predictors?

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“Machine learning”

What to include, when thousands of predictors?

“Machine learning”

(but “machine learning” can mean different things.)



Jake M. Grumbach

@JakeMGrumbach



I finally found it in real life: the consultant who runs OLS in Excel and calls it machine learning

9:17 AM · Jan 31, 2019 · Twitter for iPhone

54 Retweets **7** Quote Tweets **511** Likes



Figure 1: Don't do this.



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Figure 1: Don't do this.

If you can't describe the procedure's “learning”, it may not be “machine learning”.



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Figure 1: Don't do this.

If you can't describe the procedure's “learning”, it may not be “machine learning”.

There should probably be some testing/training, regularization,

...

Modeling Helper Functions

modelr Helper Functions

```
data(sim1)
```

```
lm_out <- lm(y ~ x, data = sim1)
```

```
tidy(lm_out)
```

```
## # A tibble: 2 x 5
```

##	term	estimate	std.error	statistic	p.value
##	<chr>	<dbl>	<dbl>	<dbl>	<dbl>
## 1	(Intercept)	4.22	0.869	4.86	4.09e- 5
## 2	x	2.05	0.140	14.7	1.17e-14

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## 1	(Intercept)	4.22	0.869	4.86	4.09e- 5
## 2	x	2.05	0.140	14.7	1.17e-14

```
glance(lm_out)
```

```
## # A tibble: 1 x 12
```

##	r.squared	adj.r.squared	sigma	statistic	p.value	df
##	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
## 1	0.885	0.880	2.20	215.	1.17e-14	1

modelr Helper Functions

Special `mutate()` functions:

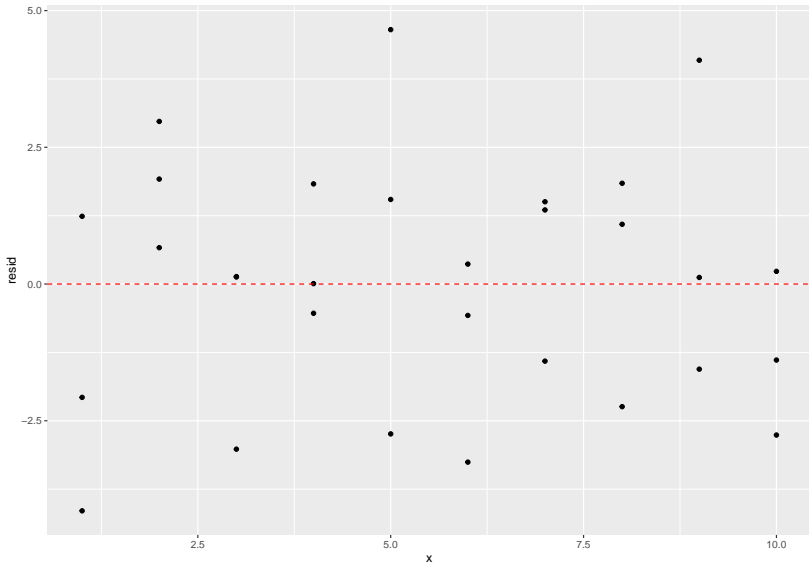
modelr Helper Functions

Special mutate() functions:

```
(sim1 <- sim1 |> add_residuals(lm_out))
```

```
## # A tibble: 30 x 3
##       x     y   resid
##   <int> <dbl> <dbl>
## 1     1     1  4.20 -2.07
## 2     1     1  7.51  1.24
## 3     1     1  2.13 -4.15
## 4     2     2  8.99  0.665
## 5     2     2 10.2   1.92
## 6     2     2 11.3   2.97
## 7     3     3  7.36 -3.02
## 8     3     3 10.5   0.130
## 9     3     3 10.5   0.136
## 10    4    12.4  0.00763
## # i 20 more rows
```

```
ggplot(sim1, aes(x, resid)) + geom_point() +  
  geom_hline(yintercept = 0, linetype = 2, color = "red")
```



modelr Helper Functions

Special mutate() functions:

```
(sim1 <- sim1 |> add_predictions(lm_out))
```

```
## # A tibble: 30 x 4
##       x     y   resid  pred
##   <int> <dbl>   <dbl> <dbl>
## 1     1     1  4.20 -2.07    6.27
## 2     1     1  7.51  1.24    6.27
## 3     1     1  2.13 -4.15    6.27
## 4     2     2  8.99  0.665   8.32
## 5     2     2 10.2   1.92   8.32
## 6     2     2 11.3   2.97   8.32
## 7     3     3  7.36 -3.02   10.4
## 8     3     3 10.5   0.130   10.4
## 9     3     3 10.5   0.136   10.4
## 10    4    12.4  0.00763 12.4
## # i 20 more rows
```


modelr Helper Functions

```
lm_out2 <- lm(y ~ x - 1, data = sim1)
```

modelr Helper Functions

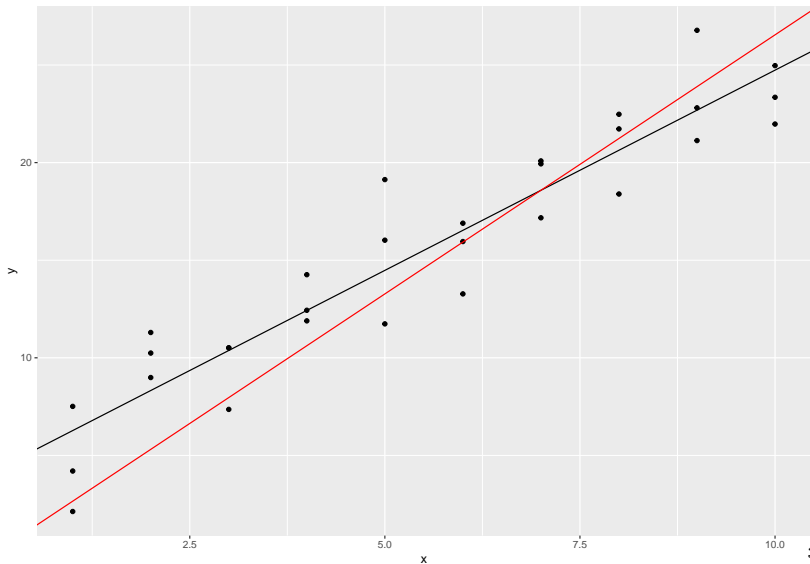
```
lm_out2 <- lm(y ~ x - 1, data = sim1)
```

```
coef(lm_out2)
```

```
##           x
```

```
## 2.654508
```

```
ggplot(sim1, aes(x, y)) + geom_point() +  
  geom_abline(intercept = coef(lm_out)[1], slope = coef(lm_out)[2]) +  
  geom_abline(intercept = 0, slope = coef(lm_out2)["x"], color = "red")
```



```
glance(lm_out)
```

```
## # A tibble: 1 x 12
##   r.squared adj.r.squared sigma statistic p.value    df
##   <dbl>         <dbl> <dbl>     <dbl>   <dbl> <dbl>
## 1     0.885         0.880   2.20     215. 1.17e-14     1
## # i 3 more variables: deviance <dbl>, df.residual <int>
```

```
glance(lm_out2)
```

```
## # A tibble: 1 x 12
##   r.squared adj.r.squared sigma statistic p.value    df
##   <dbl>         <dbl> <dbl>     <dbl>   <dbl> <dbl>
## 1     0.970         0.969   2.94      NA      NA     NA
## # i 3 more variables: deviance <dbl>, df.residual <int>
```

```
glance(lm_out)
```

```
## # A tibble: 1 x 12
##   r.squared adj.r.squared sigma statistic p.value    df
##   <dbl>         <dbl> <dbl>     <dbl>   <dbl> <dbl>
## 1     0.885         0.880   2.20     215. 1.17e-14     1
## # i 3 more variables: deviance <dbl>, df.residual <int>
```

```
glance(lm_out2)
```

```
## # A tibble: 1 x 12
##   r.squared adj.r.squared sigma statistic p.value    df
##   <dbl>         <dbl> <dbl>     <dbl>   <dbl> <dbl>
## 1     0.970         0.969   2.94      NA      NA     NA
## # i 3 more variables: deviance <dbl>, df.residual <int>
```

(R^2 and predictive quality are not the same thing ...)

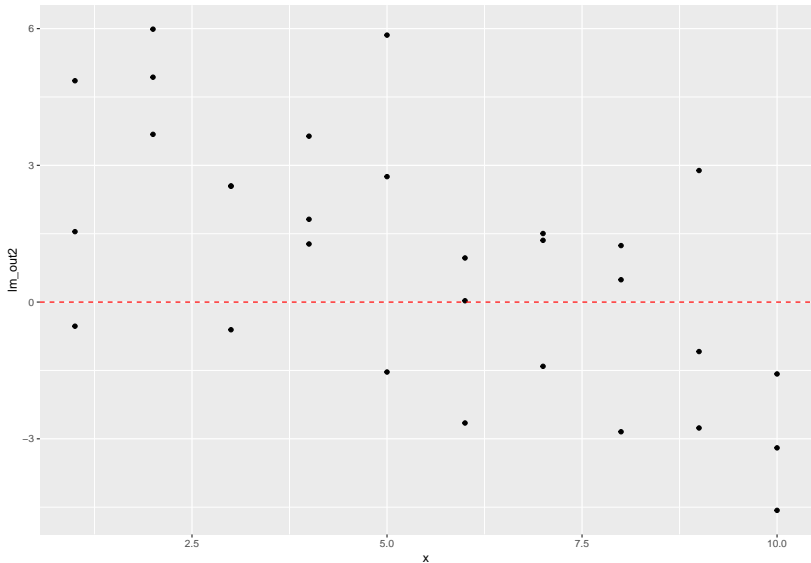
modelr Helper Functions

```
( sim1 <- sim1 |> spread_residuals(lm_out, lm_out2) )
```

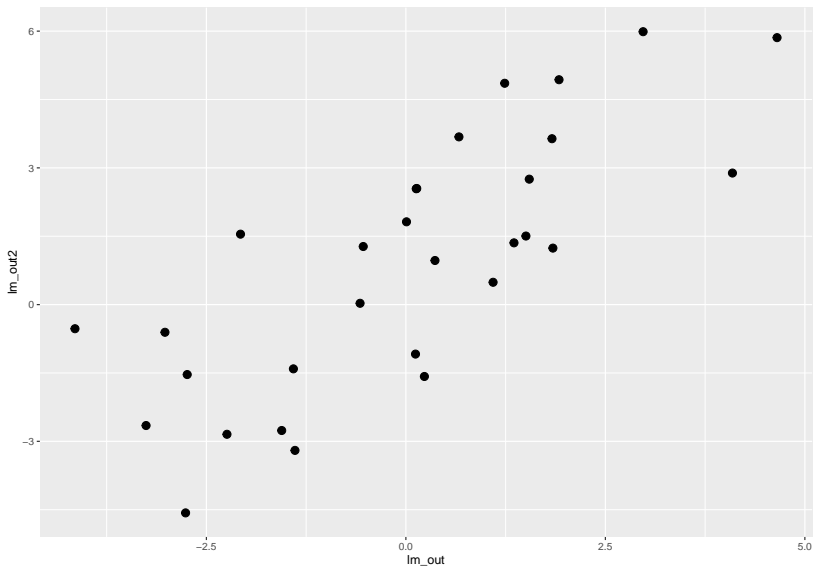
```
## # A tibble: 30 x 6
```

##		x	y	resid	pred	lm_out	lm_out2
##		<int>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
##	1	1	4.20	-2.07	6.27	-2.07	1.55
##	2	1	7.51	1.24	6.27	1.24	4.86
##	3	1	2.13	-4.15	6.27	-4.15	-0.529
##	4	2	8.99	0.665	8.32	0.665	3.68
##	5	2	10.2	1.92	8.32	1.92	4.93
##	6	2	11.3	2.97	8.32	2.97	5.99
##	7	3	7.36	-3.02	10.4	-3.02	-0.607
##	8	3	10.5	0.130	10.4	0.130	2.54
##	9	3	10.5	0.136	10.4	0.136	2.55
##	10	4	12.4	0.00763	12.4	0.00763	1.82
##	# i	20	more	rows			

```
ggplot(sim1, aes(x, lm_out2)) + geom_point() +  
  geom_hline(yintercept = 0, linetype = 2, color = "red")
```



```
ggplot(sim1, aes(lm_out, lm_out2)) + geom_point(size = 3)
```

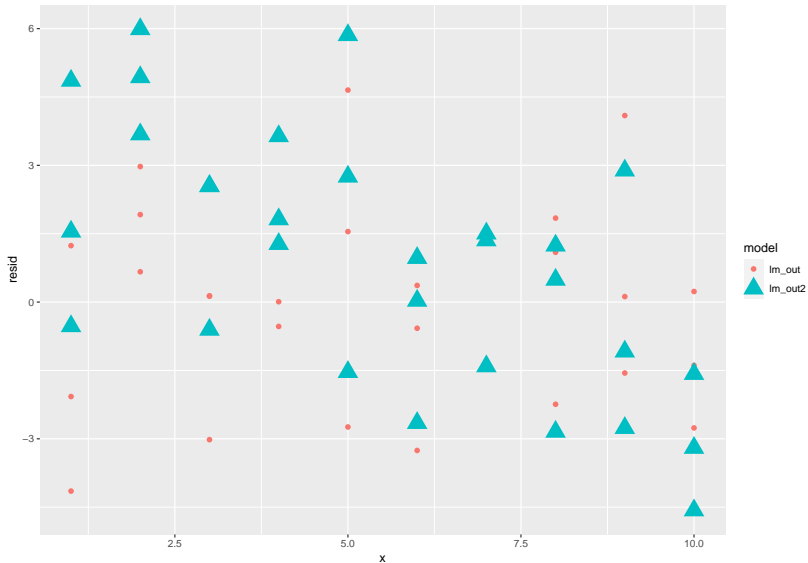


modelr Helper Functions

```
data(sim1)
( sim1 <- sim1 |> gather_residuals(lm_out, lm_out2) )
```

```
## # A tibble: 60 x 4
##   model      x      y    resid
##   <chr> <int> <dbl>   <dbl>
## 1 lm_out     1  4.20 -2.07
## 2 lm_out     1  7.51  1.24
## 3 lm_out     1  2.13 -4.15
## 4 lm_out     2  8.99  0.665
## 5 lm_out     2 10.2   1.92
## 6 lm_out     2 11.3   2.97
## 7 lm_out     3  7.36 -3.02
## 8 lm_out     3 10.5   0.130
## 9 lm_out     3 10.5   0.136
## 10 lm_out    4 12.4   0.00763
## # i 50 more rows
```

```
ggplot(sim1, aes(x, resid)) +  
  geom_point(aes(color = model, size = model, shape = model))
```



modelr Helper Functions

- ▶ `add_residuals()`
- ▶ `spread_residuals()`
- ▶ `gather_residuals()`
- ▶ `add_predictions()`
- ▶ `spread_predictions()`
- ▶ `gather_predictions()`

Other Helpers for Many Models: tidy()

```
ll <- list(lm_out, lm_out2)
```

```
ll |> map_df(tidy)
```

```
## # A tibble: 3 x 5
```

##	term	estimate	std.error	statistic	p.value
##	<chr>	<dbl>	<dbl>	<dbl>	<dbl>
## 1	(Intercept)	4.22	0.869	4.86	4.09e- 5
## 2	x	2.05	0.140	14.7	1.17e-14
## 3	x	2.65	0.0865	30.7	1.15e-23

Many Models: glance()

```
ll |> map_df(glance) |> select(1:6)
```

```
## # A tibble: 2 x 6
```

##	r.squared	adj.r.squared	sigma	statistic	p.value	
##	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
## 1	0.885	0.880	2.20	215.	1.17e-14	
## 2	0.970	0.969	2.94	NA	NA	

Many Models: glance()

```
l1 |> map_df(glance) |> select(1:6)
```

```
## # A tibble: 2 x 6
```

	r.squared	adj.r.squared	sigma	statistic	p.value	
	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
## 1	0.885	0.880	2.20	215.	1.17e-14	
## 2	0.970	0.969	2.94	NA	NA	

```
l1 |> map_df(glance) |> select(7:12)
```

```
## # A tibble: 2 x 6
```

	logLik	AIC	BIC	deviance	df.residual	nobs
	<dbl>	<dbl>	<dbl>	<dbl>	<int>	<int>
## 1	-65.2	136.	141.	136.	28	30
## 2	-74.4	153.	156.	250.	29	30

Example: `mtcars`

Machine Learning Steps

1. Feature engineering

Machine Learning Steps

1. Feature engineering: collect/create the data

Machine Learning Steps

1. Feature engineering: collect/create the data
2. Data splitting

Machine Learning Steps

1. Feature engineering: collect/create the data
2. Data splitting: split the data

Machine Learning Steps

1. Feature engineering: collect/create the data
2. Data splitting: split the data
 - ▶ Training. (80%? further split (“cross-validation”)?)
 - ▶ Validation. (for hyperparams; can be small (?))
 - ▶ Testing. (20%?)

Machine Learning Steps

1. Feature engineering: collect/create the data
2. Data splitting: split the data
 - ▶ Training. (80%? further split (“cross-validation”)?)
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3. Feature selection

Machine Learning Steps

1. Feature engineering: collect/create the data
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3. Feature selection: algorithms decide predictors to include
4. Model estimation

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4. Model estimation: find the slopes (e.g.)
5. Validation + testing

Machine Learning Steps

1. Feature engineering: collect/create the data
2. Data splitting: split the data
 - ▶ Training. (80%? further split (“cross-validation”)?)
 - ▶ Validation. (for hyperparams; can be small (?))
 - ▶ Testing. (20%?)
3. Feature selection: algorithms decide predictors to include
4. Model estimation: find the slopes (e.g.)
5. Validation + testing: evaluate preds from trained models using new data

tidymodels Example

```
library(tidymodels)
data_split <- initial_split(mtcars, prop = 2/3)

df_train <- training(data_split)
df_test  <- testing(data_split)
```

tidymodels Example

```
library(tidymodels)
data_split <- initial_split(mtcars, prop = 2/3)

df_train <- training(data_split)
df_test <- testing(data_split)
```

```
dim(df_train)
```

```
## [1] 21 11
```

```
dim(df_test)
```

```
## [1] 11 11
```

tidymodels Example

```
lm_fit <- linear_reg() |> fit(mpg ~ ., data = df_train)
lm_fit
```

```
## parsnip model object
```

```
##
```

```
##
```

```
## Call:
```

```
## stats::lm(formula = mpg ~ ., data = data)
```

```
##
```

```
## Coefficients:
```

```
## (Intercept)          cyl          disp          hp
```

```
## -52.788434      0.971688      0.012064      0.003002
```

```
##          qsec          vs          am          gear
```

```
##      1.969451     -4.052556     -0.030317      8.247851
```

tidymodels Example

```
out_preds <- bind_cols(df_test |> select(mpg),  
                        predict(lm_fit, new_data = df_test)  
                        rename(lm = .pred))
```

out_preds

##	mpg	lm
## Duster 360	14.3	11.10105
## Merc 230	22.8	31.10956
## Merc 450SL	17.3	15.27357
## Lincoln Continental	10.4	12.09299
## Honda Civic	30.4	28.05338
## Toyota Corolla	33.9	30.39759
## Toyota Corona	21.5	20.00855
## Camaro Z28	13.3	11.64362
## Porsche 914-2	26.0	34.60792
## Ford Pantera L	15.8	29.41662
## Ferrari Dino	19.7	19.64479

tidymodels Example

Next, predict with *random forest* algorithm.

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Ensemble learning algorithms:

- ▶ Boosting: models build on prior models

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tidymodels Example

Next, predict with *random forest* algorithm.

Ensemble learning algorithms:

- ▶ Boosting: models build on prior models \rightsquigarrow pick feature, predict, upweight mispredicted data, Do several times and combine.
- ▶ Bagging: (random select units, model) \rightarrow many times. No building.

tidymodels Example

Next, predict with *random forest* algorithm.

Ensemble learning algorithms:

- ▶ Boosting: models build on prior models \rightsquigarrow pick feature, predict, upweight mispredicted data, Do several times and combine.
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tidymodels Example

Next, predict with *random forest* algorithm.

Ensemble learning algorithms:

- ▶ Boosting: models build on prior models \rightsquigarrow pick feature, predict, upweight mispredicted data, Do several times and combine.
- ▶ Bagging: (random select units, model) \rightarrow many times. No building.

Random Forests are bagging algorithms.

tidymodels Example

```
rf_fit <- rand_forest(mode = "regression") |>  
  fit(mpg ~ ., data = df_train)  
rf_fit
```

```
## parsnip model object
```

```
##
```

```
## Ranger result
```

```
##
```

```
## Call:
```

```
##   ranger::ranger(x = maybe_data_frame(x), y = y, num.thre
```

```
##
```

```
## Type:                                Regression
```

```
## Number of trees:                      500
```

```
## Sample size:                          21
```

```
## Number of independent variables:      10
```

```
## Mtry:                                  3
```

```
## Target node size:                     5
```

```
## Variable importance mode:             none
```

tidymodels Example

`parsnip::rand_forest()` uses ranger engine

tidymodels Example

`parsnip::rand_forest()` uses ranger engine

There is also “Spark”.

tidymodels Example

```
out_preds <- bind_cols(out_preds,  
                        predict(rf_fit, new_data = df_test)  
                          rename(rf = .pred))
```

out_preds

##	mpg	lm	rf
## Duster 360	14.3	11.10105	15.65025
## Merc 230	22.8	31.10956	22.87099
## Merc 450SL	17.3	15.27357	15.83648
## Lincoln Continental	10.4	12.09299	13.16725
## Honda Civic	30.4	28.05338	28.26391
## Toyota Corolla	33.9	30.39759	28.68535
## Toyota Corona	21.5	20.00855	23.31111
## Camaro Z28	13.3	11.64362	16.12771
## Porsche 914-2	26.0	34.60792	25.01991
## Ford Pantera L	15.8	29.41662	18.44409
## Ferrari Dino	19.7	19.64479	20.67973

tidymodels Example

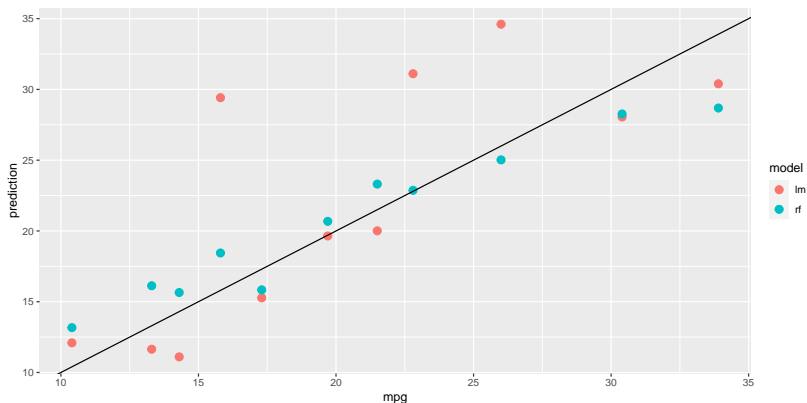
```
out_preds_long <- out_preds |>
  pivot_longer(cols = c(lm, rf),
               names_to = "model",
               values_to = "prediction")
```

```
out_preds_long
```

```
## # A tibble: 22 x 3
##       mpg model prediction
##   <dbl> <chr>      <dbl>
## 1  14.3 lm         11.1
## 2  14.3 rf         15.7
## 3  22.8 lm         31.1
## 4  22.8 rf         22.9
## 5  17.3 lm         15.3
## 6  17.3 rf         15.8
## 7  10.4 lm         12.1
## 8  10.4 rf         13.2
```

tidymodels Example

```
ggplot(out_preds_long, aes(mpg, prediction)) +  
  geom_point(aes(color = model), size = 3) +  
  geom_abline(slope = 1, intercept = 0)
```



tidymodels Example

Evaluate:

```
out_preds |> metrics(truth = mpg, estimate = lm) |>
  rename(lm = .estimate) |>
  left_join(out_preds |>
    metrics(truth = mpg, estimate = rf) |>
    rename(rf = .estimate))
```

```
## Joining with 'by = join_by(.metric, .estimator)'
```

```
## # A tibble: 3 x 4
```

```
##   .metric .estimator    lm    rf
##   <chr>   <chr>       <dbl> <dbl>
## 1 rmse    standard    5.79  2.40
## 2 rsq     standard    0.572 0.945
## 3 mae     standard    4.23  2.02
```

Example: Social Pressure Experiment (recipes)

Data Splitting

```
social <- read_csv("https://raw.githubusercontent.com/l  
  
soc_split <- initial_split(social)  
soc_train <- training(soc_split)  
soc_test <- testing(soc_split)
```

Data Splitting

```
social <- read_csv("https://raw.githubusercontent.com/l  
  
soc_split <- initial_split(social)  
soc_train <- training(soc_split)  
soc_test <- testing(soc_split)
```

```
dim(soc_train)
```

```
## [1] 229399      6
```

```
dim(soc_test)
```

```
## [1] 76467      6
```

Feature Engineering

```
social_recip <- recipe(primary2006 ~ ., data = soc_train)

social_recip
```

Feature Engineering

```
summary(social_recip)
```

```
## # A tibble: 6 x 4
##   variable      type      role      source
##   <chr>        <list>   <chr>    <chr>
## 1 sex          <chr [3]> predictor original
## 2 yearofbirth  <chr [2]> predictor original
## 3 primary2004  <chr [2]> predictor original
## 4 messages     <chr [3]> predictor original
## 5 hhsize       <chr [2]> predictor original
## 6 primary2006  <chr [2]> outcome  original
```


Feature Engineering

```
social_recip <- social_recip |>  
  step_mutate(age = 2006 - yearofbirth) |>  
  step_dummy(all_nominal(), -all_outcomes())
```

```
social_recip
```

```
##
```

```
## -- Recipe -----
```

```
##
```

```
## -- Inputs
```

```
## Number of variables by role
```

```
## outcome: 1
```

```
## predictor: 5
```

```
##
```

```
## -- Operations
```

```
## * Variable mutation for: 2006 - yearofbirth
```

```
## * Dummy variables from: all_nominal(), -all_outcomes()
```

Feature Engineering

```
social_recip <- social_recip |>  
  step_zv(all_predictors())
```

```
social_recip
```

```
##
```

```
## -- Recipe -----
```

```
##
```

```
## -- Inputs
```

```
## Number of variables by role
```

```
## outcome: 1
```

```
## predictor: 5
```

```
##
```

```
## -- Operations
```

```
## * Variable mutation for: 2006 - yearofbirth
```

```
## * Dummy variables from: all_nominal(), -all_outcomes()
```

```
## * Zero variance filter on: all_predictors()
```

Feature Engineering

```
social_recip <- social_recip |>  
  step_center(all_predictors(), -primary2004)
```

```
social_recip
```

```
##
```

```
## -- Recipe -----
```

```
##
```

```
## -- Inputs
```

```
## Number of variables by role
```

```
## outcome: 1
```

```
## predictor: 5
```

```
##
```

```
## -- Operations
```

```
## * Variable mutation for: 2006 - yearofbirth
```

```
## * Dummy variables from: all_nominal(), -all_outcomes()
```

```
## * Zero variance filter on: all_predictors()
```

```
## * Centering for: all_predictors(), -primary2004
```

Feature Engineering

```
social_recip <- social_recip |>  
  step_interact(terms = ~  
    age:all_predictors() +  
    primary2004:all_predictors()  
  )
```

Feature Engineering

Recipe complete. Time to prep and bake.

Feature Engineering

Recipe complete. Time to prep and bake.

```
social_recipe |>  
  prep()
```

```
##
```

```
## -- Recipe -----
```

```
##
```

```
## -- Inputs
```

```
## Number of variables by role
```

```
## outcome:    1
```

```
## predictor:  5
```

```
##
```

```
## Training information
```

```
soc_train_processed <- social_recip |>
  prep() |>
  bake(new_data = NULL)
```

```
soc_train_processed
```

```
## # A tibble: 229,399 x 22
```

```
##   yearofbirth primary2004 hhszize primary2006   age sex
```

```
##           <dbl>         <dbl>   <dbl>         <dbl> <dbl>
```

```
## 1           2.78             1  0.815             0 -2.78
```

```
## 2          -10.2             0 -0.185             0 10.2
```

```
## 3           27.8             1  3.81             1 -27.8
```

```
## 4           -3.22            0  1.81             0  3.22
```

```
## 5          -15.2             0 -0.185             0 15.2
```

```
## 6          -11.2             0 -1.19             1 11.2
```

```
## 7           7.78             1 -0.185             1 -7.78
```

```
## 8           22.8             1 -1.19             0 -22.8
```

```
## 9          -17.2             0 -0.185             1 17.2
```

```
## 10          -14.2            0 -0.185             0 14.2
```

```
## # i 229 389 more rows
```

```
names(soc_train_processed)
```

```
## [1] "yearofbirth" "primary2004"
## [3] "hhsize" "primary2006"
## [5] "age" "sex_male"
## [7] "messages_Control" "messages_Hawthorne"
## [9] "messages_Neighbors" "age_x_yearofbirth"
## [11] "age_x_primary2004" "age_x_hhsize"
## [13] "age_x_sex_male" "age_x_messages"
## [15] "age_x_messages_Hawthorne" "age_x_messages_Neighbors"
## [17] "yearofbirth_x_primary2004" "primary2004_x_yearofbirth"
## [19] "primary2004_x_sex_male" "primary2004_x_messages"
## [21] "primary2004_x_messages_Hawthorne" "primary2004_x_messages_Neighbors"
```

```
soc_test_processed <- social_recip |>
  prep() |>
  bake(new_data = soc_test)
```

```
soc_test_processed
```

```
## # A tibble: 76,467 x 22
```

```
##   yearofbirth primary2004 hhsz primary2006 age se
```

```
##           <dbl>         <dbl> <dbl>         <dbl> <dbl>
```

```
## 1         -5.22             0 0.815             1  5.22
```

```
## 2         -6.22             0 0.815             1  6.22
```

```
## 3          25.8             0 0.815             1 -25.8
```

```
## 4        -0.223             0 0.815             1  0.223
```

```
## 5          10.8             0 -0.185            0 -10.8
```

```
## 6        -11.2             0 -0.185            0  11.2
```

```
## 7         -7.22             0 -0.185             1  7.22
```

```
## 8        -17.2             0 -1.19             1  17.2
```

```
## 9          11.8             0 -0.185             1 -11.8
```

```
## 10         22.8             0  1.81             0 -22.8
```

```
## # i 76 467 more rows
```

Regularization Methods: LASSO, ridge regression, elastic nets

Feature Selection

- ▶ Wrappers: pick subset of covars, train on data (estimate model), test on hold-out, score predictions. Keep best-scoring subset.

Feature Selection

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- ▶ Filters: correlate covars with outcome. Keep strongest.

Feature Selection

- ▶ Wrappers: pick subset of covars, train on data (estimate model), test on hold-out, score predictions. Keep best-scoring subset.
- ▶ Filters: correlate covars with outcome. Keep strongest.
- ▶ Embeds: select features and estimate model at same time. Penalize using more predictors.

Embedded Regularization Methods

OLS reminder

Minimize SSR:

$$\arg \min_{\beta} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$
$$\arg \min_{\beta} \sum_{i=1}^n (\mathbf{y} - \mathbf{X}\hat{\beta})^2$$

Embedded Regularization Methods

L1 regularization: the LASSO (Least Absolute Shrinkage and Selection Operator)

$$\arg \min_{\beta} \left[\sum_{i=1}^n \left(y_i - \mathbf{X} \hat{\beta} \right)^2 + \lambda \sum_{j=1}^k |\hat{\beta}_j| \right]$$

Embedded Regularization Methods

L1 regularization: the LASSO (Least Absolute Shrinkage and Selection Operator)

$$\arg \min_{\beta} \left[\sum_{i=1}^n \left(y_i - \mathbf{X}\hat{\beta} \right)^2 + \lambda \sum_{j=1}^k |\hat{\beta}_j| \right]$$

L2 regularization: Ridge regression

$$\arg \min_{\beta} \left[\sum_{i=1}^n \left(y_i - \mathbf{X}\hat{\beta} \right)^2 + \lambda \sum_{j=1}^k \hat{\beta}_j^2 \right]$$

Embedded Regularization Methods

Mix L1 and L2: Elastic net

$$\arg \min_{\beta} \left(\frac{\sum_{i=1}^n (y_i - \mathbf{X}\hat{\beta})^2}{2n} + \lambda \left[\alpha \sum_{j=1}^k |\hat{\beta}_j| + \frac{1-\alpha}{2} \sum_{j=1}^k \hat{\beta}_j^2 \right] \right)$$

Embedded Regularization Methods

Mix L1 and L2: Elastic net

$$\arg \min_{\beta} \left(\frac{\sum_{i=1}^n (y_i - \mathbf{X}\hat{\beta})^2}{2n} + \lambda \left[\alpha \sum_{j=1}^k |\hat{\beta}_j| + \frac{1-\alpha}{2} \sum_{j=1}^k \hat{\beta}_j^2 \right] \right)$$

Regularized trees, ...

R packages for Regularization, etc.

- ▶ `glmnet`

- ▶ `caret`

See also `tidymodels`, `parsnip`, ...

References

Breiman, Leo. 2001. “Statistical Modeling: The Two Cultures (with comments and a rejoinder by the author).” *Statistical Science* 16 (3): 199–231.
<https://doi.org/10.1214/ss/1009213726>.