

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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1. Generative modeling
2. Predictive modeling

Breiman (2001b)

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

Which predictors should I include?

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Helpful?

- ▶ Affect outcome
- ▶ 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
```

modelr Helper Functions

```
glance(lm_out) |> select(1:5)
```

```
## # A tibble: 1 x 5
##   r.squared adj.r.squared sigma statistic p.value
##   <dbl>         <dbl> <dbl>      <dbl>    <dbl>
## 1    0.885         0.880  2.20      215.  1.17e-14
```

```
glance(lm_out) |> select(6:12)
```

```
## # A tibble: 1 x 7
##       df logLik   AIC   BIC deviance df.residual  nobs
##   <dbl> <dbl> <dbl> <dbl>    <dbl>      <int> <int>
## 1     1  -65.2  136.  141.    136.         28    30
```

modelr Helper Functions

Special `mutate()` functions:

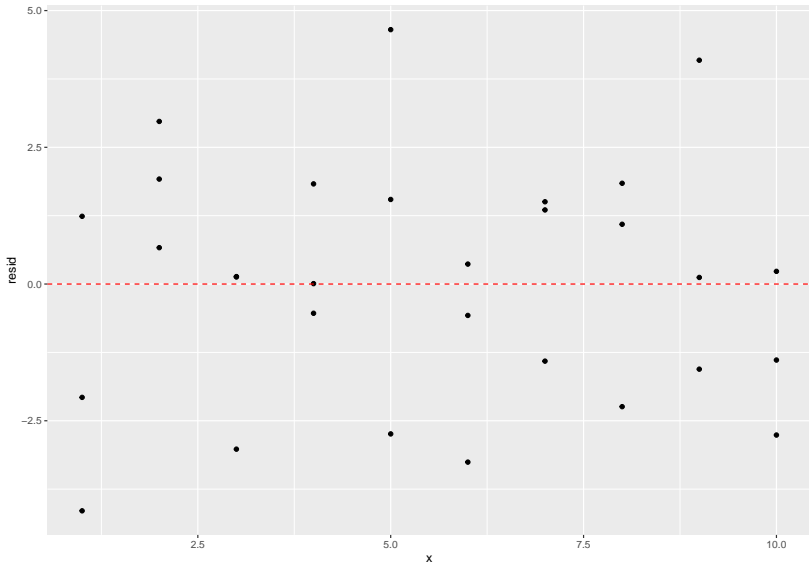
modelr Helper Functions

Special mutate() functions:

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

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

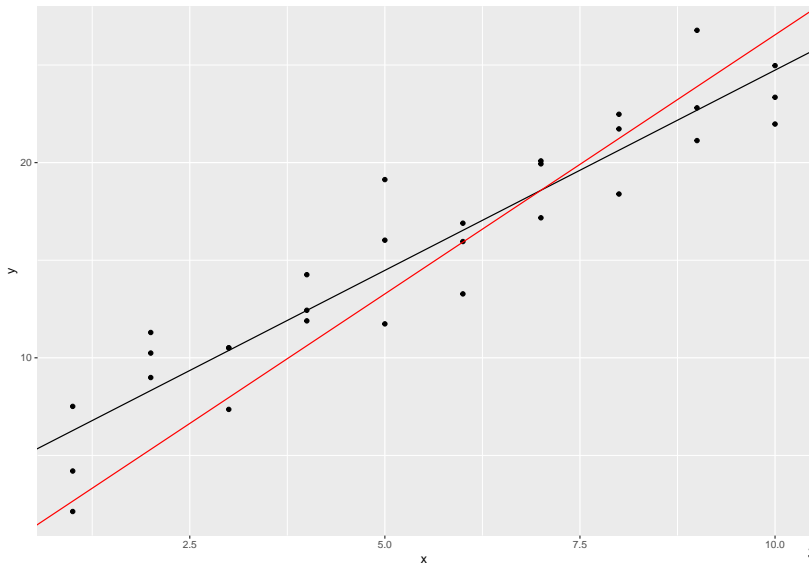
```
lm_out2 <- lm(y ~ x - 1, data = sim1)
```

```
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      943. 1.15e-23     1
## # 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     943. 1.15e-23     1
## # i 3 more variables: deviance <dbl>, df.residual <int>
```

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

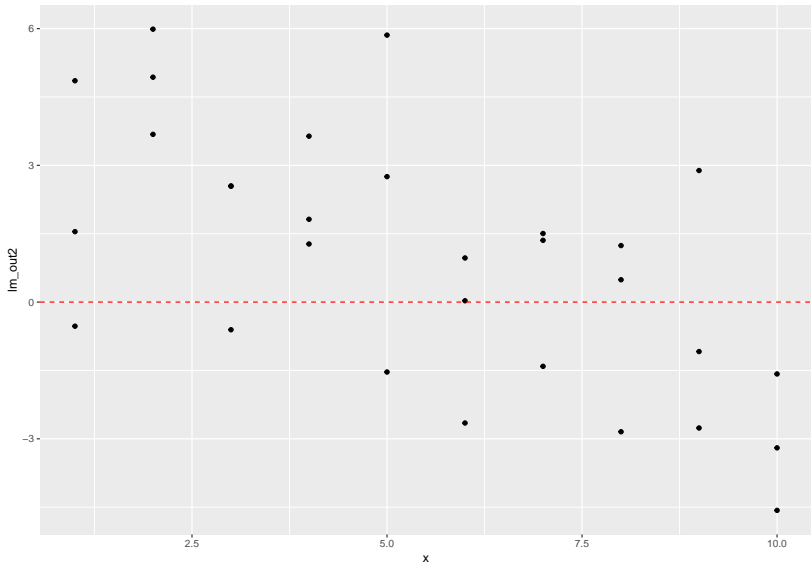
modelr Helper Functions

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

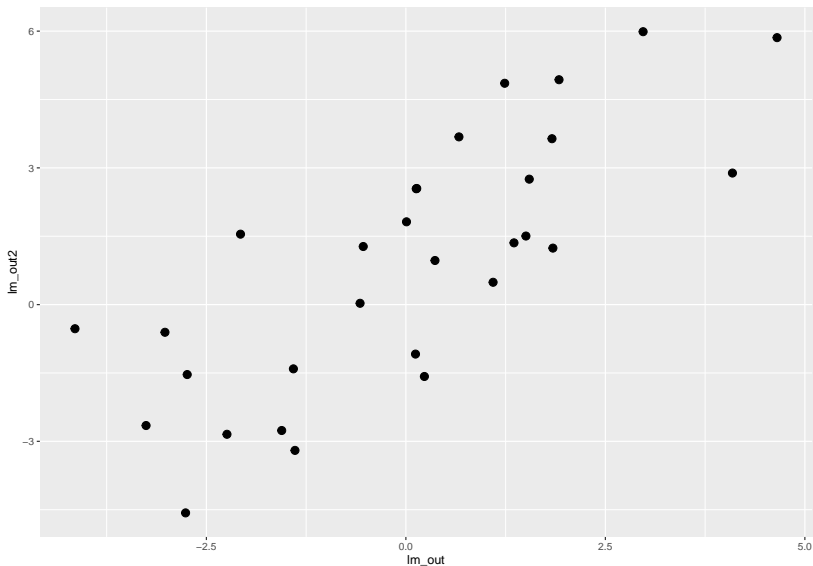
```
## # A tibble: 30 x 6
```

##		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)
```

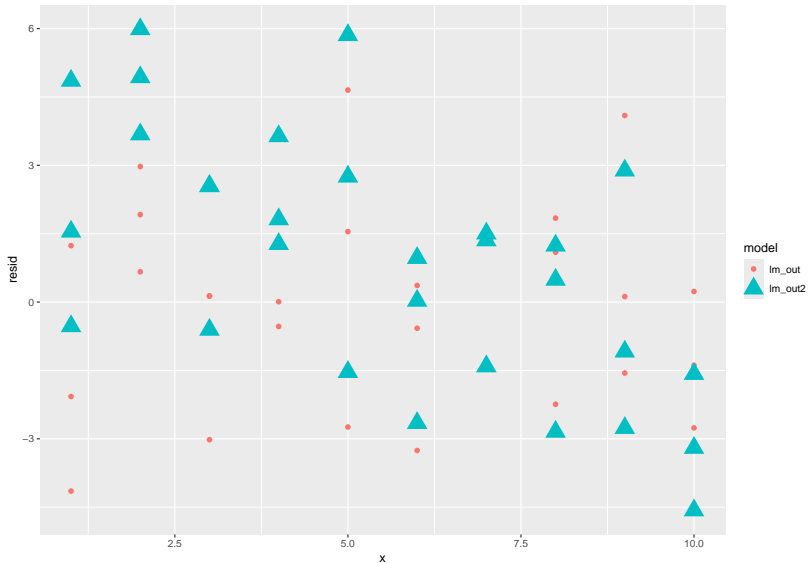


modelr Helper Functions

```
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(1:5)
```

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

##	r.squared	adj.r.squared	sigma	statistic	p.value
##	<dbl>	<dbl>	<dbl>	<dbl>	<dbl>
## 1	0.885	0.880	2.20	215.	1.17e-14
## 2	0.970	0.969	2.94	943.	1.15e-23

Many Models: glance()

```
ll |> map_df(glance) |> select(1:5)
```

```
## # A tibble: 2 x 5
##   r.squared adj.r.squared sigma statistic p.value
##   <dbl>      <dbl> <dbl>      <dbl>      <dbl>
## 1    0.885        0.880  2.20        215. 1.17e-14
## 2    0.970        0.969  2.94        943. 1.15e-23
```

```
ll |> map_df(glance) |> select(6:12)
```

```
## # A tibble: 2 x 7
##       df logLik   AIC   BIC deviance df.residual  nobs
##   <dbl> <dbl> <dbl> <dbl>     <dbl>      <int> <int>
## 1     1 -65.2  136.  141.     136.         28    30
## 2     1 -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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4. Model estimation

Machine Learning Steps

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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

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
## -3.07537	-0.19100	0.02830	-0.02431
## qsec	vs	am	gear
## 0.53145	-0.51353	1.54036	3.84550

tidymodels Example

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

out_preds

##	mpg	lm
## Mazda RX4 Wag	21.0	21.66514
## Hornet 4 Drive	21.4	20.20164
## Hornet Sportabout	18.7	18.80151
## Merc 450SE	16.4	13.48582
## Cadillac Fleetwood	10.4	14.11564
## Lincoln Continental	10.4	13.17200
## Toyota Corolla	33.9	28.64901
## Fiat X1-9	27.3	27.68602
## Porsche 914-2	26.0	30.67169
## Ford Pantera L	15.8	25.50938
## Ferrari Dino	19.7	19.95970

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.
- ▶ 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.
- ▶ Bagging: (random select units, model) \rightarrow many times. No building.

Random Forests are bagging algorithms.

Breiman (2001a)

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
## Mazda RX4 Wag	21.0	21.66514	20.36497
## Hornet 4 Drive	21.4	20.20164	19.52452
## Hornet Sportabout	18.7	18.80151	16.45822
## Merc 450SE	16.4	13.48582	16.42280
## Cadillac Fleetwood	10.4	14.11564	16.26746
## Lincoln Continental	10.4	13.17200	15.78517
## Toyota Corolla	33.9	28.64901	29.41605
## Fiat X1-9	27.3	27.68602	29.41278
## Porsche 914-2	26.0	30.67169	25.27119
## Ford Pantera L	15.8	25.50938	17.23360
## Ferrari Dino	19.7	19.95970	19.91055

tidymodels Example

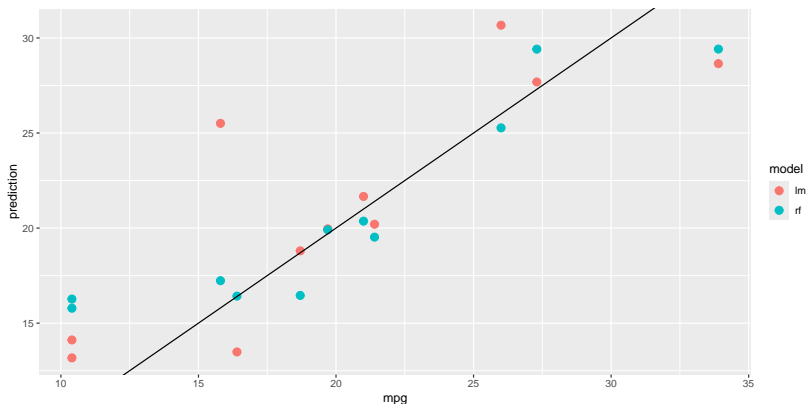
```
out_preds_long <- out_preds |>  
  pivot_longer(cols = c(lm, rf),  
               names_to = "model",  
               values_to = "prediction")
```

```
out_preds_long
```

```
## # A tibble: 22 x 3  
##       mpg model prediction  
##   <dbl> <chr>      <dbl>  
## 1   21    lm        21.7  
## 2   21    rf        20.4  
## 3  21.4    lm        20.2  
## 4  21.4    rf        19.5  
## 5  18.7    lm        18.8  
## 6  18.7    rf        16.5  
## 7  16.4    lm        13.5  
## 8  16.4    rf        16.4
```

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	4.00	3.01
## 2	rsq	standard	0.683	0.842
## 3	mae	standard	2.88	2.27

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      -13.2              1 -0.185              0 13.2
```

```
## 2       0.779              1 -0.185              0 -0.779
```

```
## 3      -6.22              1 -0.185              0  6.22
```

```
## 4      -4.22              0  0.815              0  4.22
```

```
## 5      -5.22              1 -1.18              1  5.22
```

```
## 6     -19.2              0  0.815              0 19.2
```

```
## 7     -25.2              0 -0.185              1 25.2
```

```
## 8     -29.2              0 -0.185              1 29.2
```

```
## 9     -12.2              0  0.815              0 12.2
```

```
## 10     -4.22              0  0.815              0  4.22
```

```
## # 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 hhszize primary2006   age sex
```

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

```
## 1         -15.2             0 -0.185             0  15.2
```

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

```
## 3          10.8             0 -0.185             0 -10.8
```

```
## 4         -15.2             1 -1.18             1  15.2
```

```
## 5          12.8             1 -1.18             0 -12.8
```

```
## 6          10.8             1 -0.185             1 -10.8
```

```
## 7          26.8             0  1.82             0 -26.8
```

```
## 8           8.78             0 -0.185             0  -8.78
```

```
## 9         -24.2             0 -0.185             0  24.2
```

```
## 10          2.78             0 -0.185             0  -2.78
```

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

Now, with train and test data ready, add *model specification, fitting, evaluation, deployment* to workflow.

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

- ▶ 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.

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. 2001a. “Random Forests.” *Machine Learning* 45: 5–32.
- . 2001b. “Statistical Modeling: The Two Cultures.” *Statistical Science* 16 (3): 199–215.
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