

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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 - (novel theory, prior theory, prior findings)

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(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”

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- ▶ 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?

What to include, when thousands of predictors?

“Machine learning”

What to include, when thousands of predictors?

“Machine learning”

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



Jake M. Grumbach

@JakeMGrumbach

ooo

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:

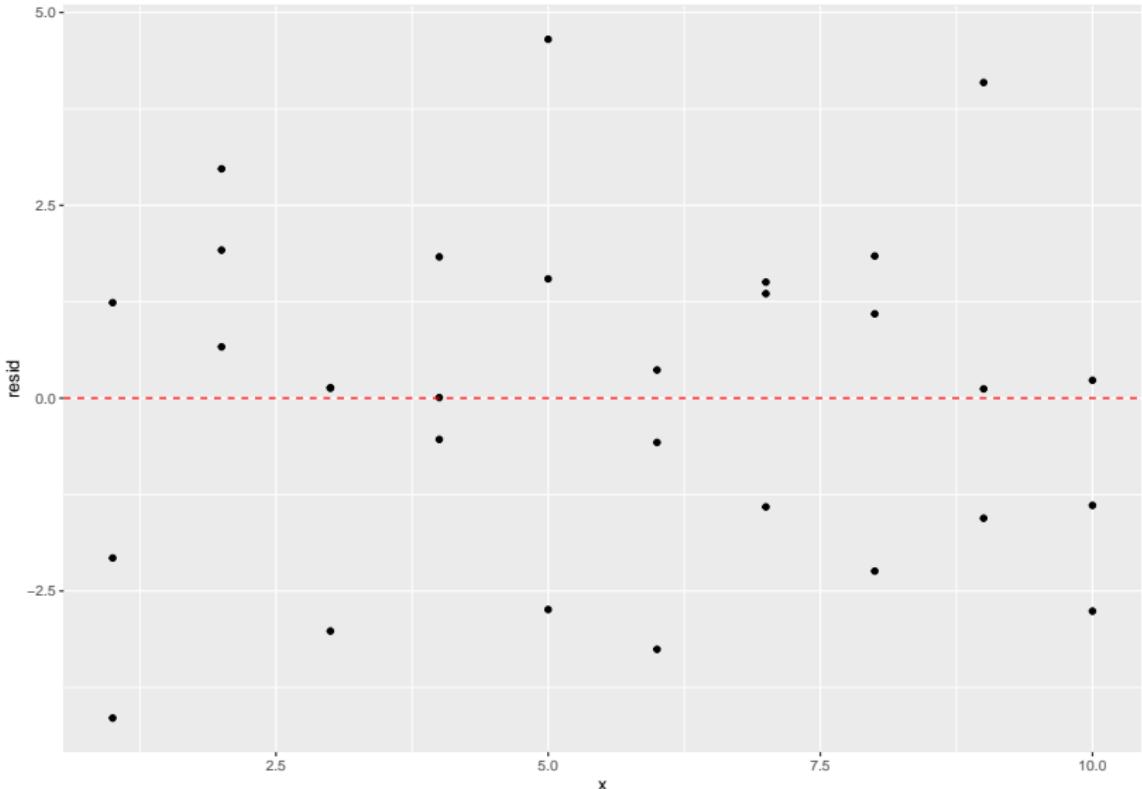
modelr Helper Functions

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   4.20 -2.07    6.27
## 2     1   7.51  1.24    6.27
## 3     1   2.13 -4.15    6.27
## 4     2   8.99  0.665   8.32
## 5     2  10.2   1.92    8.32
## 6     2  11.3   2.97    8.32
## 7     3   7.36 -3.02   10.4
## 8     3  10.5   0.130   10.4
## 9     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)
```

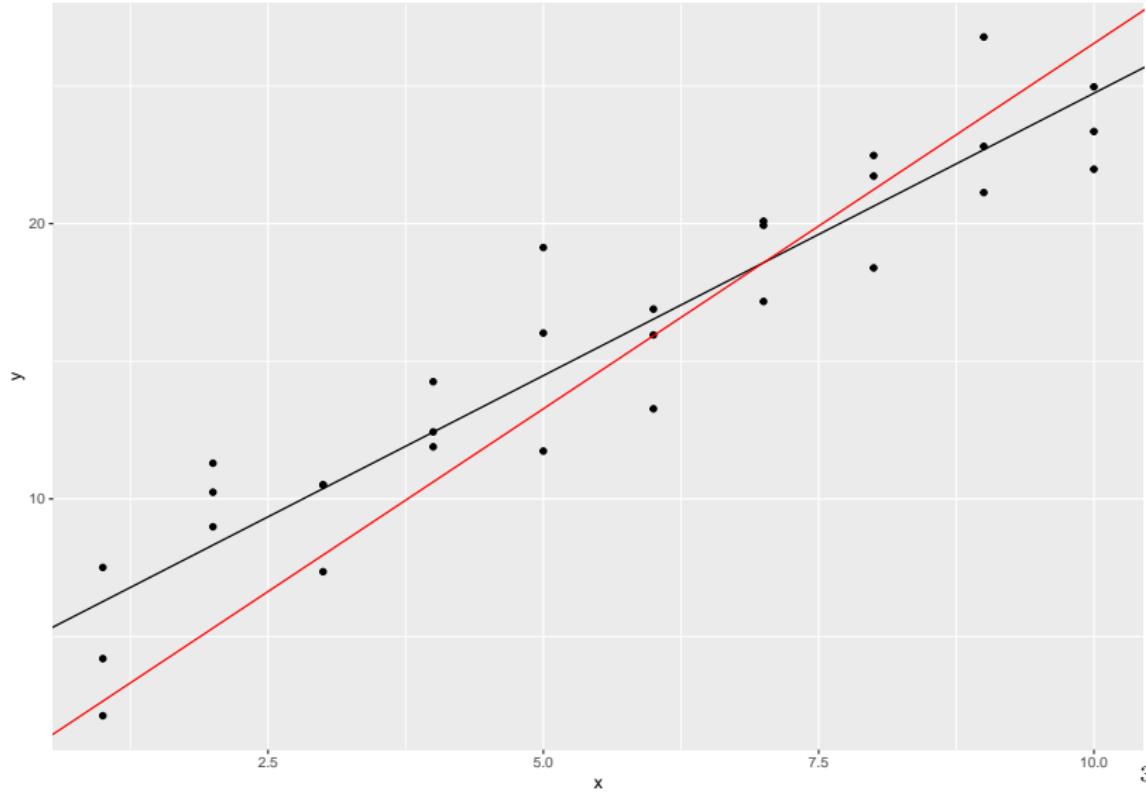
modelr Helper Functions

```
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)
```

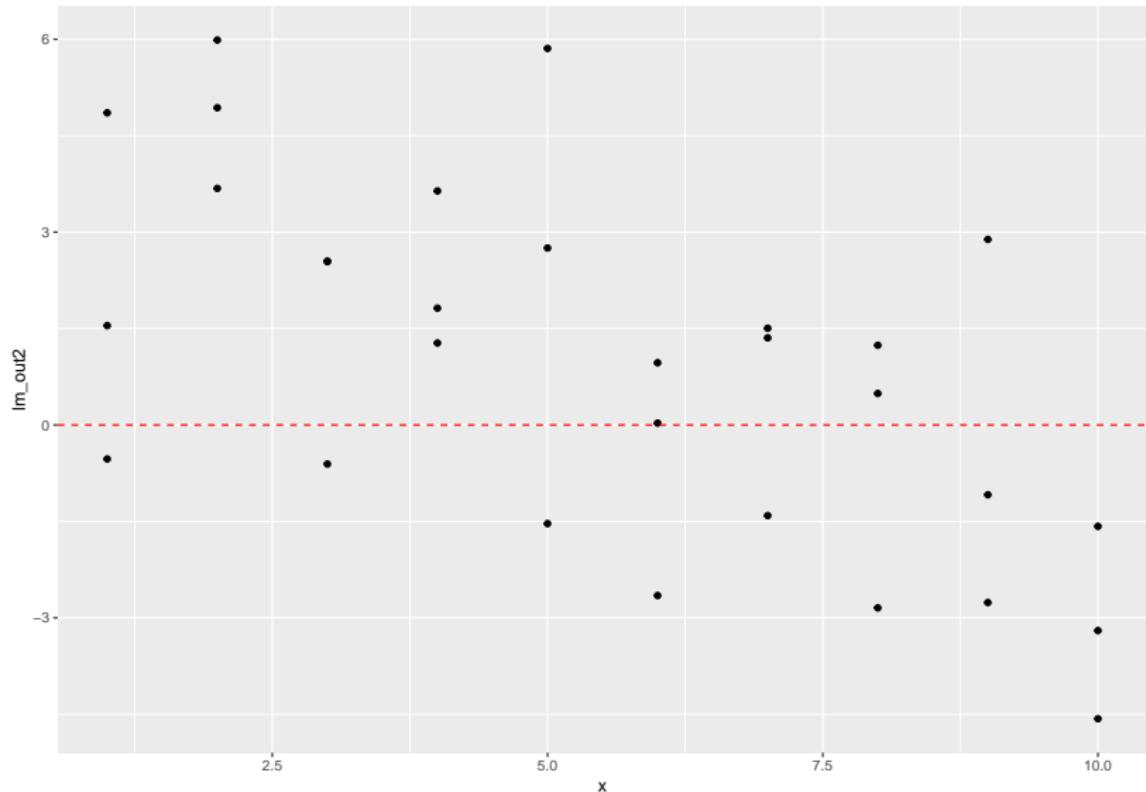
```
## # A tibble: 1 x 12
##   r.squared adj.r.squared sigma statistic p.value    df
##       <dbl>          <dbl>  <dbl>      <dbl>    <dbl>  <dbl>
## 1     0.970          0.969  2.94      943. 1.15e-23 1
## # i 3 more variables: deviance <dbl>, df.residual <int>
```

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

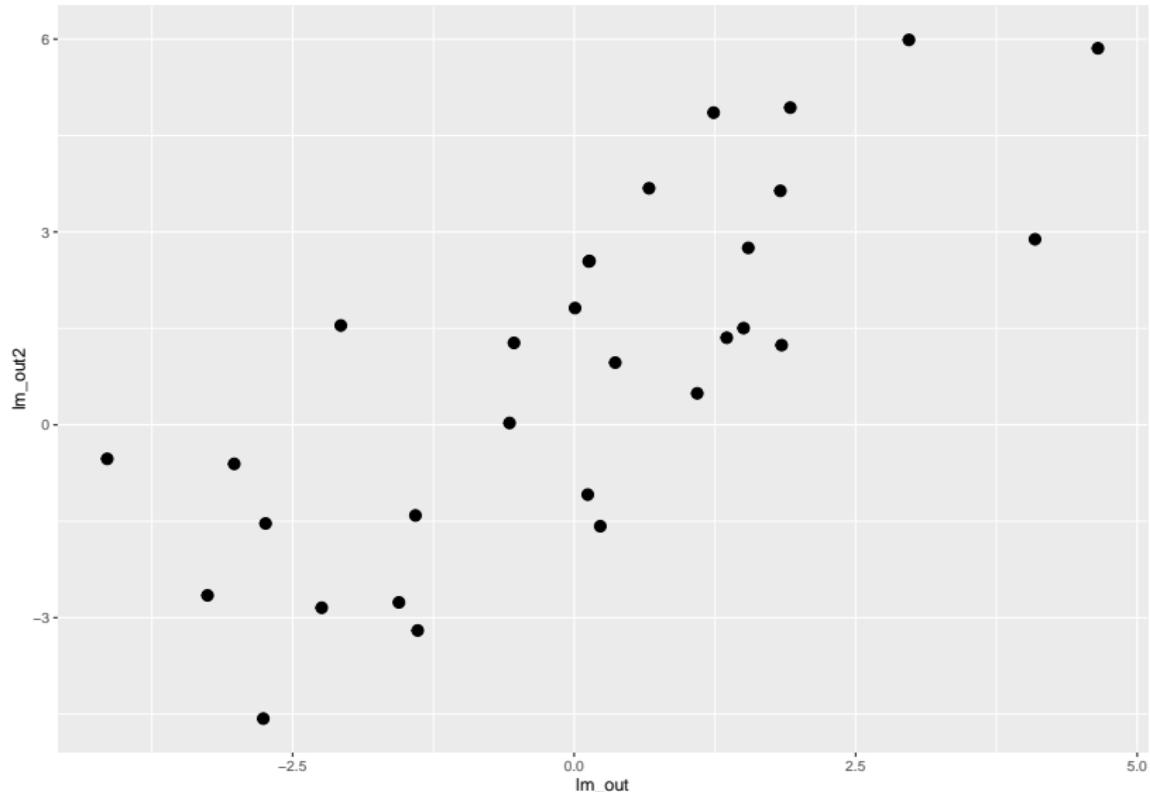
modelr Helper Functions

```
( 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)
```

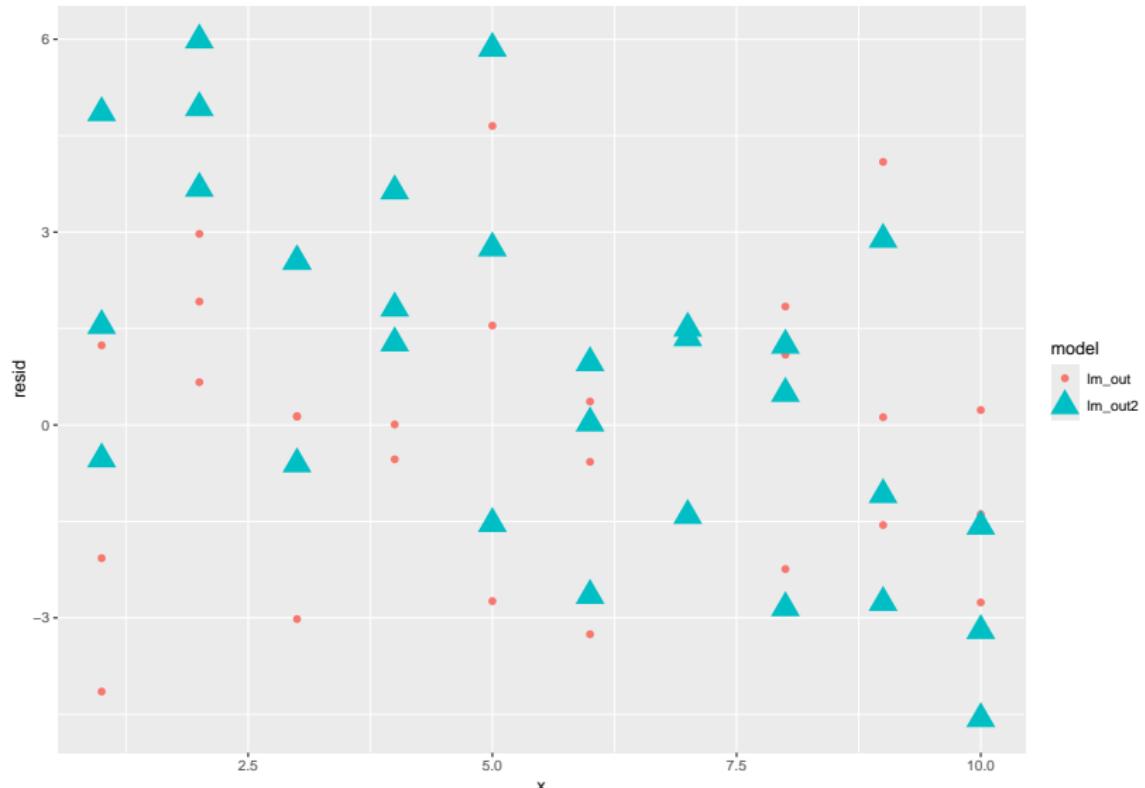


modelr Helper Functions

```
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()

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

11 |> 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)
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```
## # 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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 - ▶ Testing. (20%?)
3. Feature selection

Machine Learning Steps

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3. Feature selection: algorithms decide predictors to include
4. Model estimation: find the slopes (e.g.)

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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

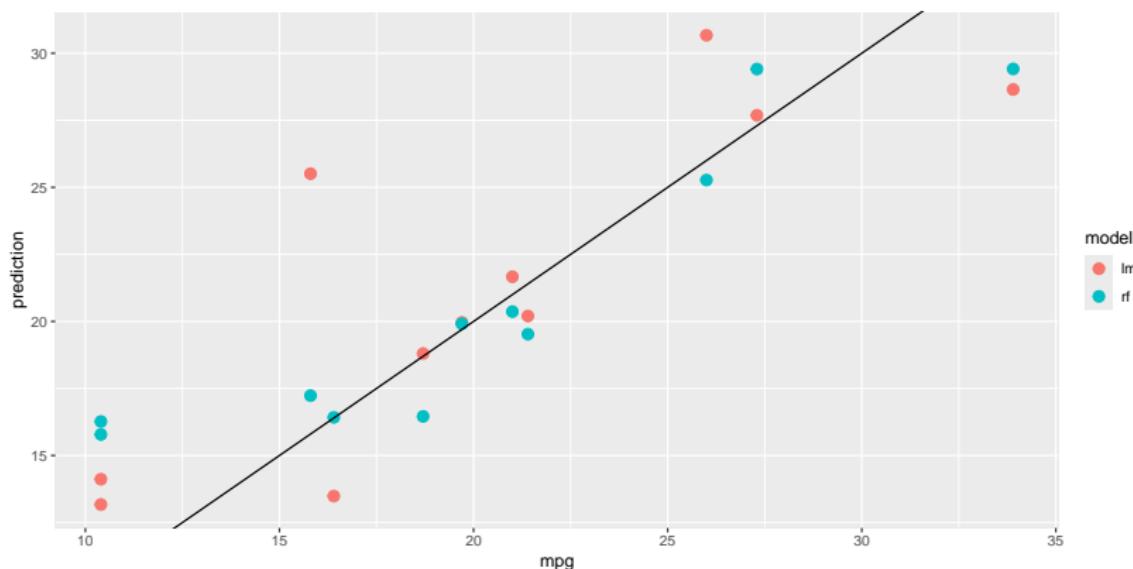
```
out_preds_long <- out_preds |>  
  pivot_longer(cols = c(lm, rf),  
               names_to = "model",  
               values_to = "prediction")
```

```
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/lmkoval/ML4DS/master/datasets/social.csv")  
  
soc_split <- initial_split(social)  
soc_train <- training(soc_split)  
soc_test <- testing(soc_split)
```

Data Splitting

```
social <- read_csv("https://raw.githubusercontent.com/
```

```
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_recip |>  
  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 hhszie primary2006      age sex
##   <dbl>        <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] "hhszie"               "primary2006"
## [5] "age"                  "sex_male"
## [7] "messages_Control"     "messages_Hawthorne"
## [9] "messages_Neighbors"    "age_x_yearofbirth"
## [11] "age_x_primary2004"    "age_x_hhszie"
## [13] "age_x_sex_male"        "age_x_messages"
## [15] "age_x_messages_Hawthorne" "age_x_messages_Neighbors"
## [17] "yearofbirth_x_primary2004" "primary2004_x_primary2006"
## [19] "primary2004_x_sex_male"   "primary2004_x_sex_female"
## [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 hhszie primary2006      age sex
##   <dbl>        <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      -10.8
## 4 -15.2          1 -1.18       15.2
## 5 12.8           1 -1.18      -12.8
## 6 10.8           1 -0.185      -10.8
## 7 26.8           0  1.82       -26.8
## 8 8.78            0 -0.185      -8.78
## 9 -24.2          0 -0.185      24.2
## 10 2.78           0 -0.185     -2.78
## # i 76,457 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

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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)

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

Embedded Regularization Methods

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

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

L2 regularization: Ridge regression

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

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.
<http://www.jstor.org/stable/2676681>.