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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Breiman (2001)

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- Raw data
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- Specification searching
  (repeat modeling with same data)
- Training and testing
  (repeat modeling, different data)

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  (No omitted variable bias)

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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
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- 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.)

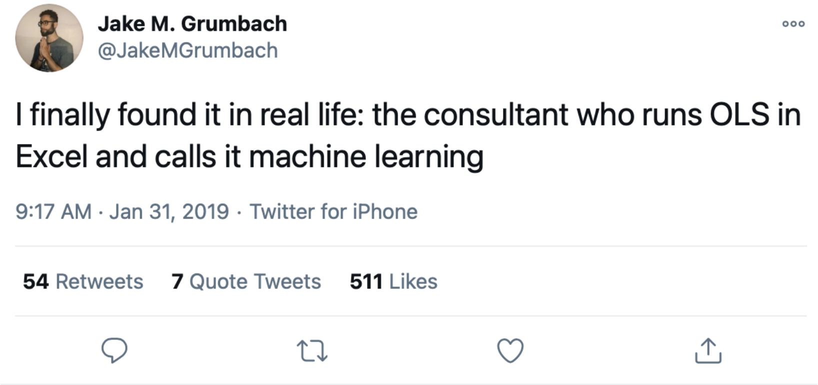

Figure 1: Don't do this.

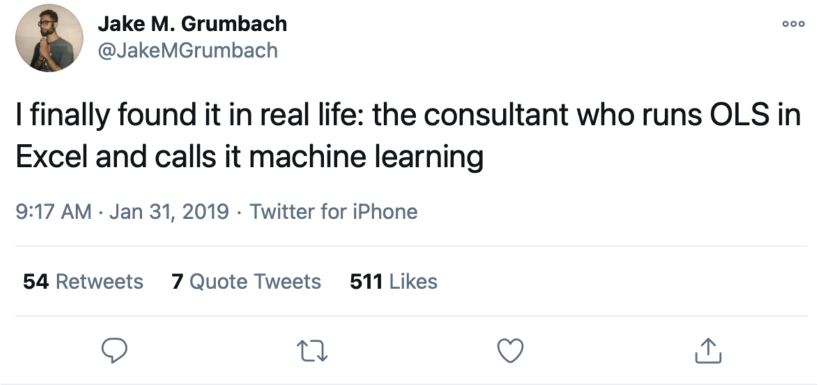

Figure 1: Don't do this.

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

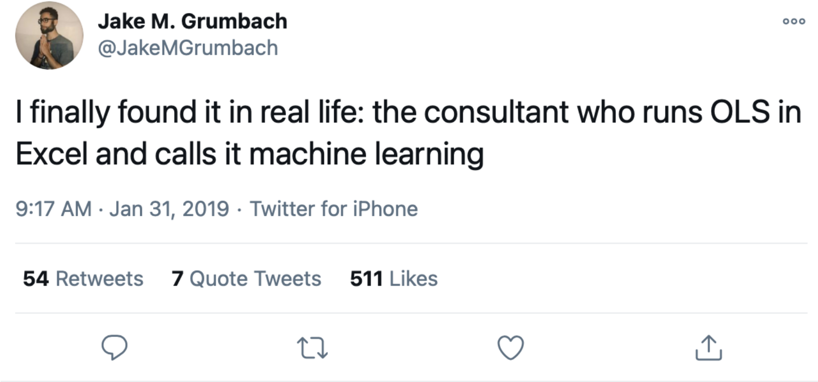

Figure 1: Don't do this.

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

```r
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
```

```r
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:

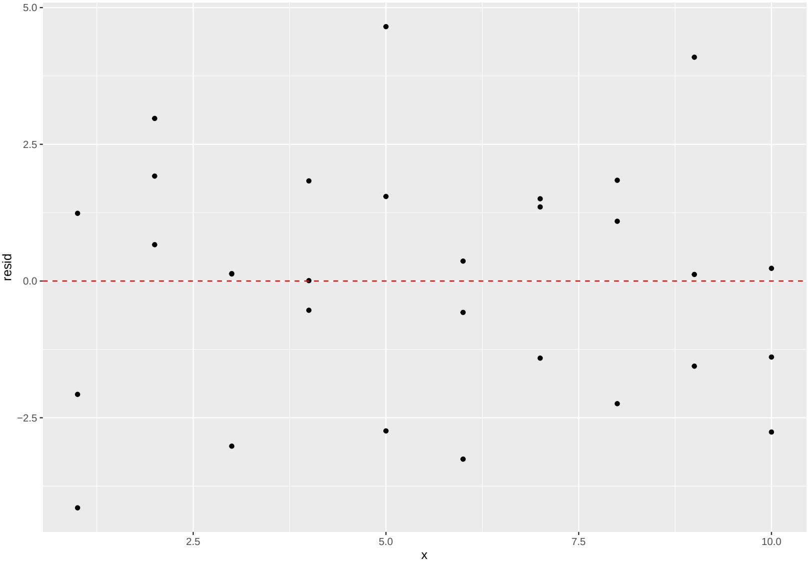
modelr Helper Functions

Special mutate() functions:

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

```
## # A tibble: 30 x 3
##         x     y    resid
##     <int> <dbl>    <dbl>
##  1      1  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
```

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



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

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

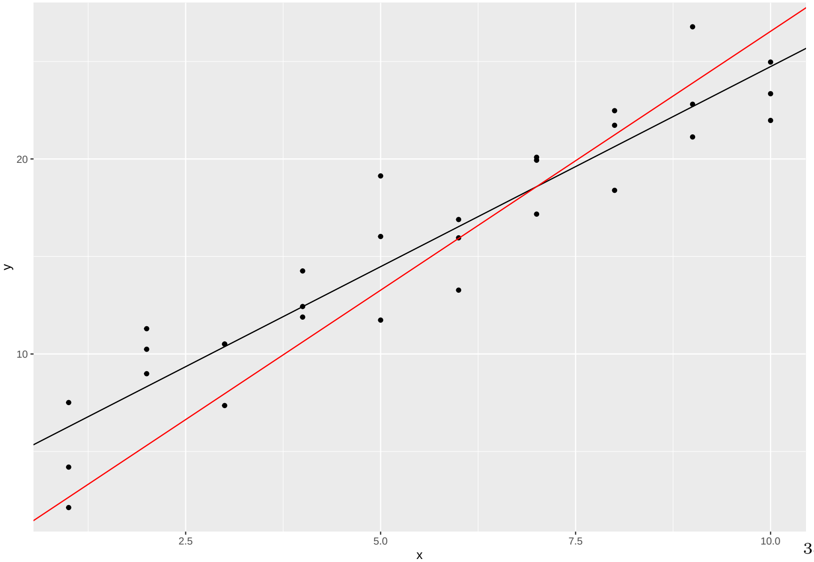
modelr Helper Functions

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

```r
coef(lm_out2)
```

```
##        x
## 2.654508
```

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



```r
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>,
```

```r
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
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>,
```

```r
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>,
```

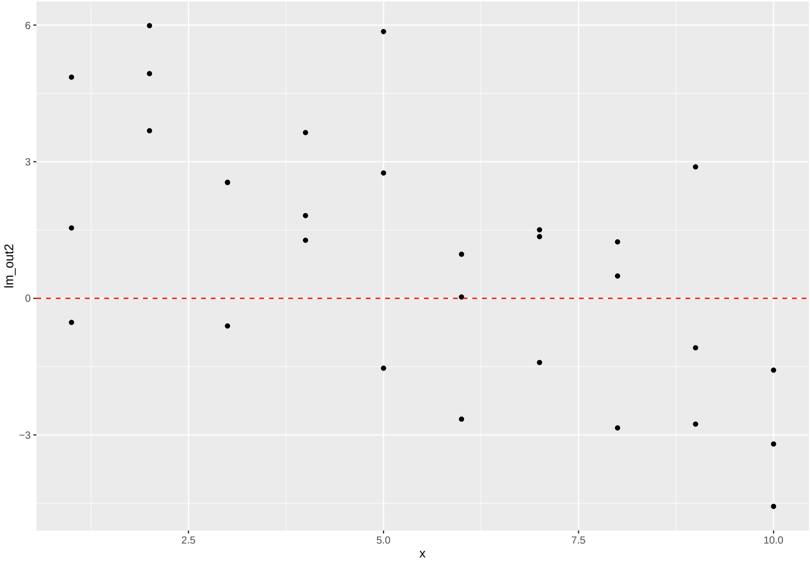
(R^2 and predictive quality are not the same thing . . .)

`modelr` Helper Functions

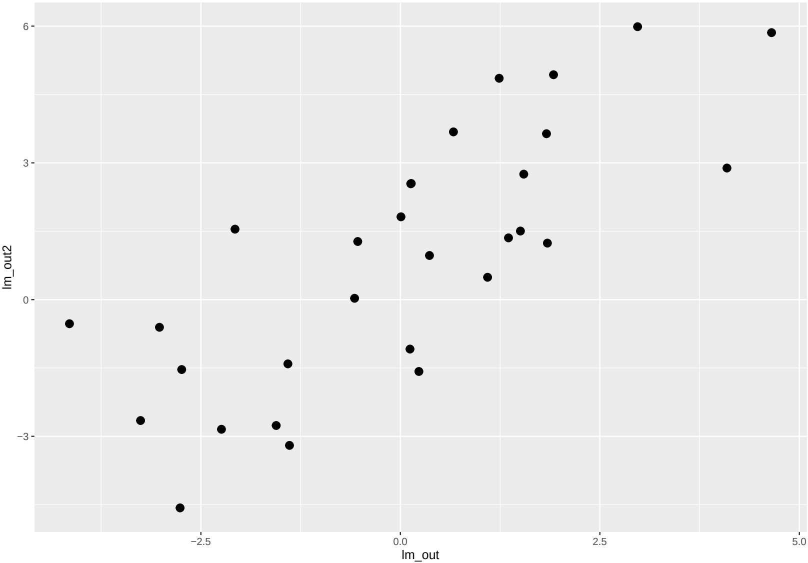
```
( sim1 <- sim1 |> spread_residuals(lm_out, lm_out2) )
```

```
## # 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
```

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



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

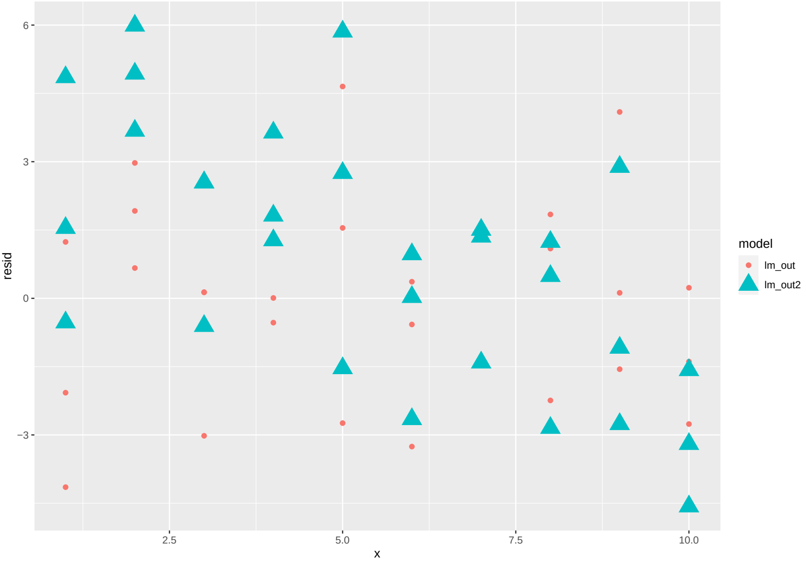


modelr Helper Functions

```
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
```

```r
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()

```r
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    d
##       <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          N
```

Many Models: glance()

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

```
## # A tibble: 2 x 6
##   r.squared adj.r.squared sigma statistic   p.value    d
##       <dbl>         <dbl> <dbl>     <dbl>     <dbl> <db
## 1     0.885         0.880  2.20      215.  1.17e-14
## 2     0.970         0.969  2.94       NA  NA          N
```

```r
ll |> 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

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2. Data splitting: split the data

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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

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3. Feature selection

Machine Learning Steps

1. Feature engineering: collect/create the data
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- Testing. (20%?)

3. Feature selection: algorithms decide predictors to include
4. Model estimation

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

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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

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

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

```r
dim(df_train)
```

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

```r
dim(df_test)
```

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

tidymodels Example

```r
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
##  -127.13656      3.24904      0.01493      0.06491
##        qsec           vs           am         gear
##     4.21793     -3.09021           NA     10.66257
```

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         21.0 17.68862
## Mazda RX4 Wag     21.0 18.87465
## Hornet 4 Drive    21.4 18.42586
## Hornet Sportabout 18.7 19.98952
## Merc 240D         24.4 21.63137
## Merc 230          22.8 37.74679
## Merc 280C         17.8 22.20879
## Toyota Corona     21.5 19.32277
## Porsche 914-2     26.0 33.08862
## Ford Pantera L    15.8 39.18207
## Maserati Bora     15.0 24.66780
```

`tidymodels` Example

Next, predict with *random forest* algorithm.

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Ensemble learning algorithms:

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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

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

```
##                      mpg       lm       rf
## Mazda RX4           21.0 17.68862 20.45133
## Mazda RX4 Wag       21.0 18.87465 20.36097
## Hornet 4 Drive      21.4 18.42586 18.54591
## Hornet Sportabout   18.7 19.98952 16.77318
## Merc 240D           24.4 21.63137 21.83636
## Merc 230            22.8 37.74679 21.47683
## Merc 280C           17.8 22.20879 19.54339
## Toyota Corona       21.5 19.32277 22.28518
## Porsche 914-2       26.0 33.08862 25.05484
## Ford Pantera L      15.8 39.18207 17.33194
## Maserati Bora       15.0 24.66780 16.16053
```

tidymodels Example

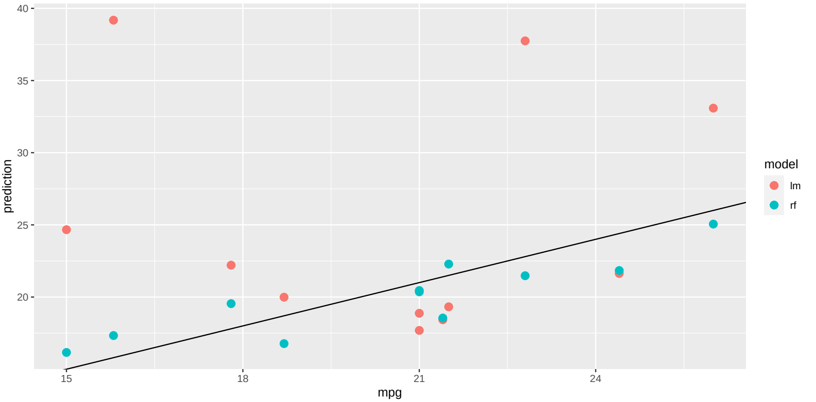
```
out_preds_long <- out_preds |>
  pivot_longer(cols = c(lm, rf),
               names_to = "model",
               values_to = "prediction")

out_preds_long
```

```
## # A tibble: 22 x 3
##      mpg model prediction
##    <dbl> <chr>      <dbl>
##  1  21   lm          17.7
##  2  21   rf          20.5
##  3  21   lm          18.9
##  4  21   rf          20.4
##  5  21.4 lm          18.4
##  6  21.4 rf          18.5
##  7  18.7 lm          20.0
##  8  18.7 rf          16.8
```

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   9.40     1.63
## 2 rsq     standard   0.000476 0.783
## 3 mae     standard   6.74     1.46
```

Example: Social Pressure Experiment (`recipes`)

Data Splitting

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

soc_split <- initial_split(social)
soc_train <- training(soc_split)
soc_test <- testing(soc_split)
```

Data Splitting

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

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())
```

```r
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())
```

```r
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.

```r
social_recip |>
  prep()
```

```
##
## -- Recipe ------------------------------------------
##
## -- Inputs
## Number of variables by role
## outcome:   1
## predictor: 5
##
## -- Training information
```

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

soc_train_processed
```

```
## # A tibble: 229,399 x 22
##    yearofbirth primary2004 hhsize primary2006     age se
##          <dbl>       <dbl>  <dbl>       <dbl>   <dbl>
##  1     -19.2             0 -0.184           0  19.2
##  2      -8.21            1 -0.184           1   8.21
##  3      19.8             1 -0.184           1 -19.8
##  4      -6.21            0 -0.184           1   6.21
##  5       3.79            0 -0.184           1  -3.79
##  6      11.8             0 -1.18            0 -11.8
##  7       0.793           0 -0.184           0  -0.793
##  8       4.79            1  0.816           1  -4.79
##  9       7.79            0 -0.184           1  -7.79
## 10      -1.21            1 -0.184           0   1.21
## # i 229,389 more rows
```

```r
names(soc_train_processed)
```

```
##  [1] "yearofbirth"                       "primary2004
##  [3] "hhsize"                            "primary2006
##  [5] "age"                               "sex_male"
##  [7] "messages_Control"                  "messages_Ha
##  [9] "messages_Neighbors"                "age_x_yearo
## [11] "age_x_primary2004"                 "age_x_hhsiz
## [13] "age_x_sex_male"                    "age_x_messa
## [15] "age_x_messages_Hawthorne"          "age_x_messa
## [17] "yearofbirth_x_primary2004"         "primary2004
## [19] "primary2004_x_sex_male"            "primary2004
## [21] "primary2004_x_messages_Hawthorne" "primary2004
```

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

soc_test_processed
```

```
## # A tibble: 76,467 x 22
##    yearofbirth primary2004 hhsize primary2006    age sex
##          <dbl>       <dbl>  <dbl>       <dbl>  <dbl>
##  1      -15.2            0 -0.184           0  15.2
##  2       11.8            0 -0.184           0 -11.8    -
##  3       10.8            0 -0.184           0 -10.8
##  4        4.79           1 -0.184           1  -4.79
##  5      -13.2            0 -1.18            1  13.2    -
##  6      -17.2            0 -1.18            1  17.2
##  7       -2.21           0  1.82            0   2.21
##  8       -7.21           1 -0.184           0   7.21
##  9        6.79           0 -0.184           0  -6.79
## 10        2.79           0 -1.18            0  -2.79   -
## # i 76,457 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

- 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:

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

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

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

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

Embedded Regularization Methods

Mix L1 and L2: Elastic net

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

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.