Concepts in Machine Learning
Winter Institute in Data Science

Ryan T. Moore

2023-01-09

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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  (novel theory, prior theory, prior findings)

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  (novel theory, prior theory, prior findings)
- Raw data
  ("data look nonlinear, so $\ldots + \beta x^2 + \ldots$")
- Specification searching
  (repeat modeling with same data)
- Testing and training
  (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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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.)

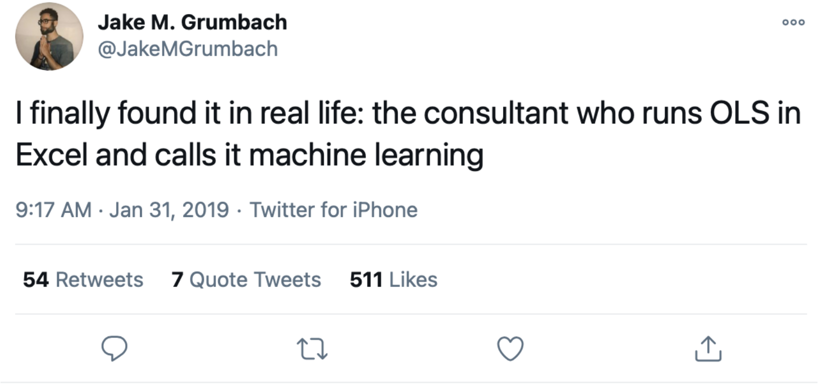

Figure 1: Don't do this.

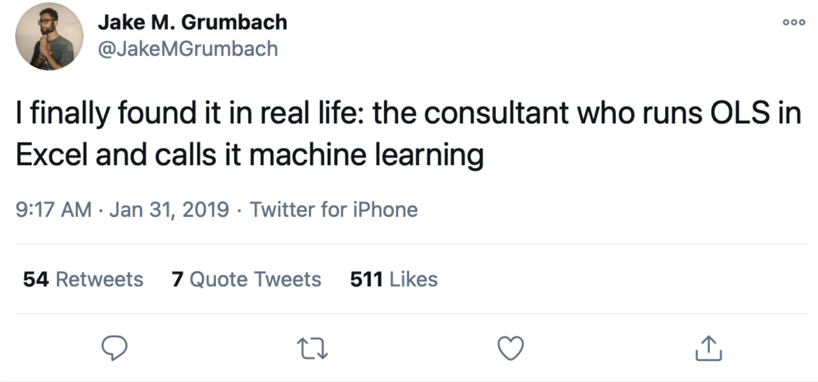

Figure 1: Don't do this.

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

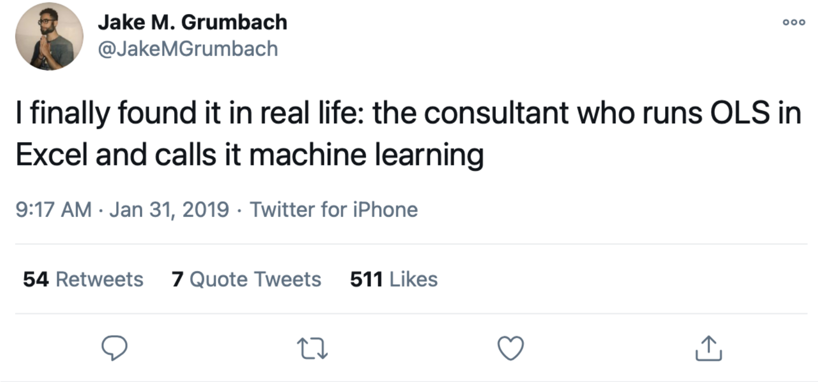

Figure 1: Don't do this.

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
```

modelr Helper Functions

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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.squa~1 sigma stati~2  p.value    df lo
##       <dbl>        <dbl> <dbl>   <dbl>    <dbl> <dbl>  <
## 1     0.885        0.880  2.20    215. 1.17e-14     1  -
## # ... with 2 more variables: df.residual <int>, nobs <in
```

`modelr` Helper Functions

Special `mutate()` functions:

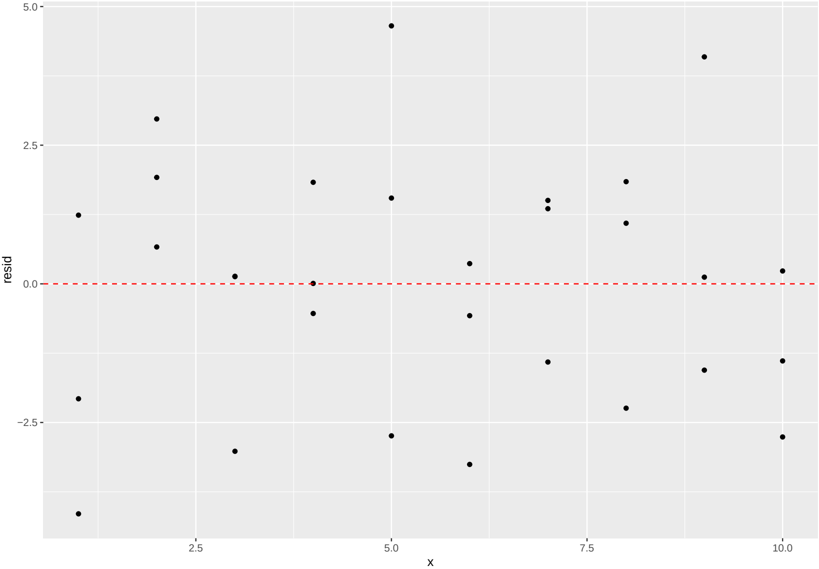
modelr Helper Functions

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
## # ... with 20 more rows
```

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



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
## # ... with 20 more rows
```

`modelr` Helper Functions

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

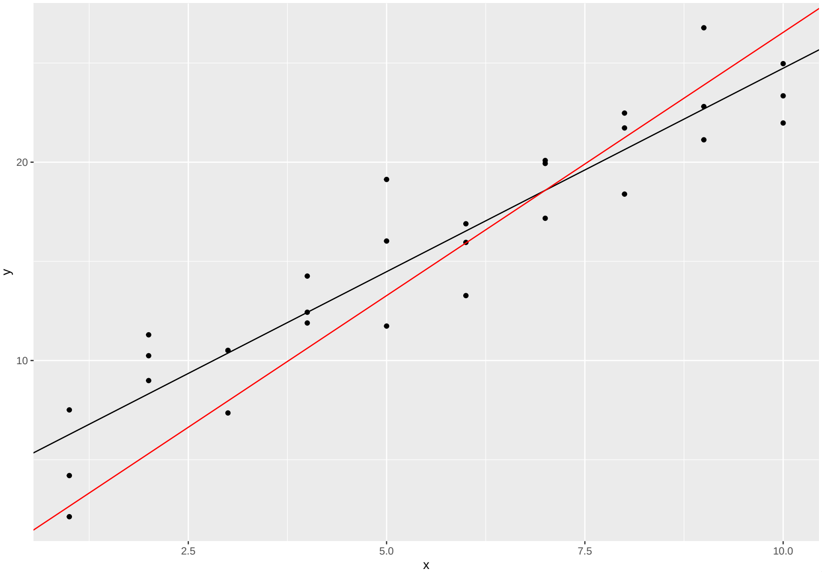
modelr Helper Functions

```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
```

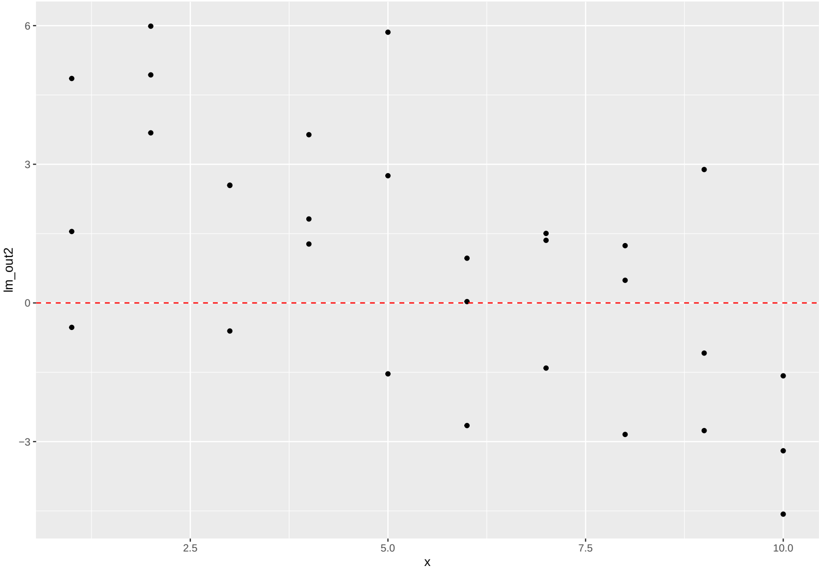


modelr Helper Functions

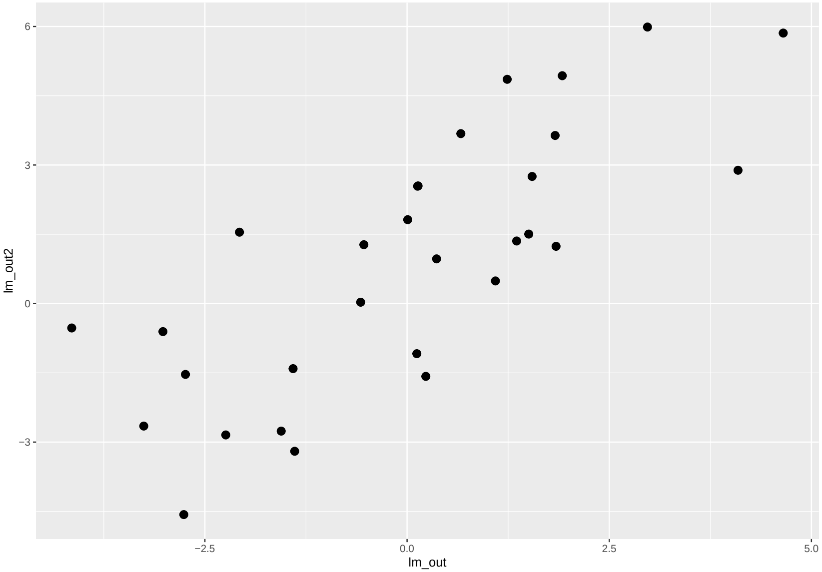
```
( sim1 <- sim1 %>% spread_residuals(lm_out, lm_out2) )
```

```
## # 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
## # ... with 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)
```

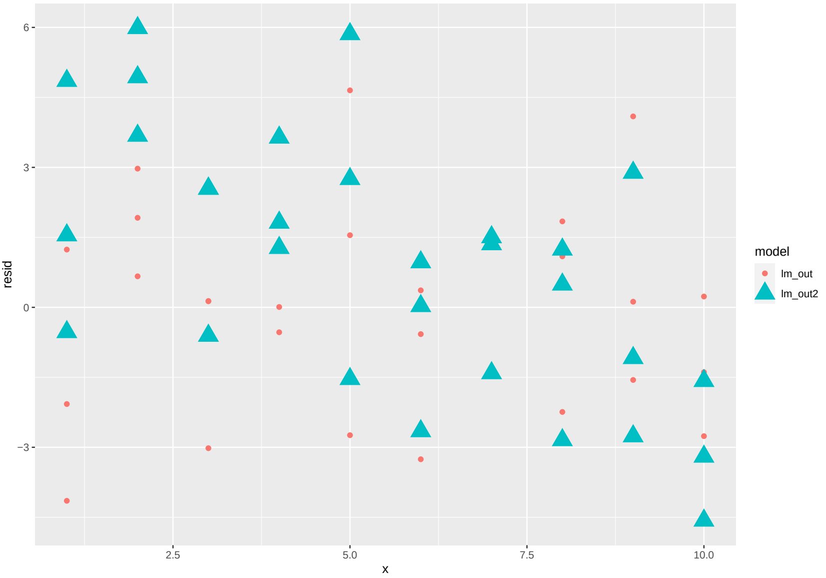


modelr Helper Functions

```
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
## # ... with 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()`

```
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    c
##       <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
```

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
```

```
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 the data

Machine Learning Steps

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

Machine Learning Steps

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Machine Learning Steps

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- Training. (80%? further split ("cross-validation")?)
- Validation. (for hyperparams; can be small (?))
- Testing. (20%?)

Machine Learning Steps

1. Feature engineering: collect 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

Machine Learning Steps

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

- Training. (80%? further split ("cross-validation")?)
- Validation. (for hyperparams; can be small (?))
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3. Feature selection: algorithms decide predictors to include

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4. Model estimation

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2. Data splitting: split the data

- Training. (80%? further split ("cross-validation")?)
- Validation. (for hyperparams; can be small (?))
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Machine Learning Steps

1. Feature engineering: collect 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

tidymodels Example

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

data_train <- training(data_split)
data_test <- testing(data_split)
```

tidymodels Example

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

data_train <- training(data_split)
data_test <- testing(data_split)
```

```r
dim(data_train)
```

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

```r
dim(data_test)
```

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

tidymodels Example

```
lm_fit <- linear_reg() %>% fit(mpg ~ ., data = data_train)
lm_fit
```

```
## parsnip model object
##
##
## Call:
## stats::lm(formula = mpg ~ ., data = data)
##
## Coefficients:
## (Intercept)          cyl         disp           hp
##    35.88207     -1.05411     -0.00762      0.02137
##        qsec           vs           am         gear
##     0.45523      0.30930      2.71692     -1.78824
```

tidymodels Example

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

```
##                   mpg       lm
## Datsun 710       22.8 28.95529
## Valiant          18.1 22.21417
## Duster 360       14.3 17.00604
## Merc 240D        24.4 22.24034
## Merc 450SLC      15.2 17.35224
## Honda Civic      30.4 29.84949
## Toyota Corona    21.5 28.17302
## AMC Javelin      15.2 18.12251
## Camaro Z28       13.3 16.02768
## Pontiac Firebird 19.2 16.46137
## Fiat X1-9        27.3 30.00786
```

`tidymodels` Example

Next, predict with *random forest* algorithm.

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

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Ensemble learning algorithms:

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`tidymodels` Example

Next, predict with *random forest* algorithm.

Ensemble learning algorithms:

- Boosting: models build on prior models
- 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 = data_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 = data_test
                         rename(rf = .pred))
out_preds
```

```
##                    mpg       lm       rf
## Datsun 710        22.8 28.95529 28.10413
## Valiant           18.1 22.21417 20.30823
## Duster 360        14.3 17.00604 15.47055
## Merc 240D         24.4 22.24034 23.78722
## Merc 450SLC       15.2 17.35224 15.92268
## Honda Civic       30.4 29.84949 29.64706
## Toyota Corona     21.5 28.17302 25.71693
## AMC Javelin       15.2 18.12251 17.47906
## Camaro Z28        13.3 16.02768 15.58399
## Pontiac Firebird  19.2 16.46137 16.88390
## Fiat X1-9         27.3 30.00786 30.10763
```

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, by = c(".metric", ".estimator")

## # A tibble: 3 x 4
##   .metric .estimator    lm    rf
##   <chr>   <chr>      <dbl> <dbl>
## 1 rmse    standard   3.66  2.65
## 2 rsq     standard   0.741 0.857
## 3 mae     standard   3.24  2.24
```

Example: Social Pressure Experiment (`recipes`)

Data Splitting

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

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

Data Splitting

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

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

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

social_recip
```

```
## Recipe
##
## Inputs:
##
##       role #variables
##    outcome          1
##  predictor          5
```

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

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

```
social_recip
```

```
## Recipe
##
## Inputs:
##
##       role #variables
##    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:
##
##       role #variables
##    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

```r
social_recip <- social_recip %>%
  step_center(all_predictors(), -primary2004)
```

```r
social_recip
```

```
## Recipe
##
## Inputs:
##
##       role #variables
##    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()
                )
```

```
social_recip
```

```
## Recipe
##
## Inputs:
##
##       role #variables
##    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
## Interactions with age:all_predictors() + primary2004
```

Feature Engineering

Recipe complete. Time to prep and bake.

Feature Engineering

Recipe complete. Time to prep and bake.

```
social_recip %>%
  prep()
```

```
## Recipe
##
## Inputs:
##
##       role #variables
##    outcome          1
##  predictor          5
##
## Training data contained 229399 data points and no mi
##
## Operations:
##
## Variable mutation for ~2006 - yearofbirth [trained]
```

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

soc_train_processed
```

```
## # A tibble: 229,399 x 22
##    yearofbirth primary2~1 hhsize prima~2   age sex_m~3
##          <dbl>      <dbl>  <dbl>   <dbl> <dbl>   <dbl>
##  1       9.77           1 -0.184       1 -9.77   0.499
##  2      24.8            0 -0.184       0 -24.8  -0.501
##  3       3.77           0 -0.184       1 -3.77   0.499
##  4      20.8            0 -0.184       0 -20.8  -0.501
##  5      -0.228          0 -0.184       0  0.228 -0.501
##  6     -16.2            0  0.816       1  16.2  -0.501
##  7      17.8            1 -0.184       1 -17.8   0.499
##  8      -1.23           0  1.82        0  1.23   0.499
##  9      -0.228          0 -0.184       0  0.228 -0.501
## 10      -5.23           1 -0.184       0  5.23  -0.501
## # ... with 229,389 more rows, 13 more variables: age_x_y
```

```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 primary2~1 hhsize prima~2    age sex_m~3
##          <dbl>      <dbl>  <dbl>   <dbl>  <dbl>   <dbl>
##  1      -6.23           0  0.816       1   6.23   -0.501
##  2      24.8            0  0.816       0 -24.8     0.499
##  3      -0.228          0  0.816       1   0.228   0.499
##  4      12.8            1 -1.18        0 -12.8    -0.501
##  5      10.8            1 -0.184       1 -10.8    -0.501
##  6     -13.2            0 -1.18        1  13.2    -0.501
##  7      22.8            0  1.82        0 -22.8     0.499
##  8       8.77           0 -0.184       0  -8.77    0.499
##  9       8.77           0 -0.184       0  -8.77   -0.501
## 10      12.8            0 -1.18        0 -12.8     0.499
## # ... with 76,457 more rows, 13 more variables: age_x_ye
```

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.

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- 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:

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

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.