How to Make a Predictive Model

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Homework 6 notes

Remember to **connect with the claim**: what point was the author making?

- Get as *close to the source* as you can
  - e.g., "Our World in Data" is great, but often data is pre-wrangled. See "Source" tab.
- *tidy data tip*: Try expressing your data as a bunch of simple sentences, one per observation.
  - On January 22, the number of Covid cases in Afghanistan was 0.
  - On January 23, the number of Covid cases in Afghanistan was 0.
  - ...
- For bar charts, use `geom_col` (not `geom_bar`) unless you know exactly what you're doing.
- If you're having trouble getting data, talk with me!

Recap: regression error measures

- MAE: mean absolute error
- MSE: mean *squared* error

Units

- If sale price is in $'s, what *units* is MAE in?
- MSE?
- What unit would the square root of MSE (RMSE) be in?

Q&A

> Should I look at (root) mean squared error, mean absolute error, or what?

Think: Would I use the mean or the median to summarize the errors?

- If the model is mostly good but makes a few large errors, is that bad (use MSE!), or does it mean we should probably ignore those points as outliers (use MAE!).
- For a single number: **Median** minimizes MAE. **Mean** minimizes MSE. (Think: what would minimize max *absolute* error?)
- Most *models* try to minimize MSE. (but that doesn't mean *you* have to.)

A nice discussion, including concrete examples, here.

Q&A

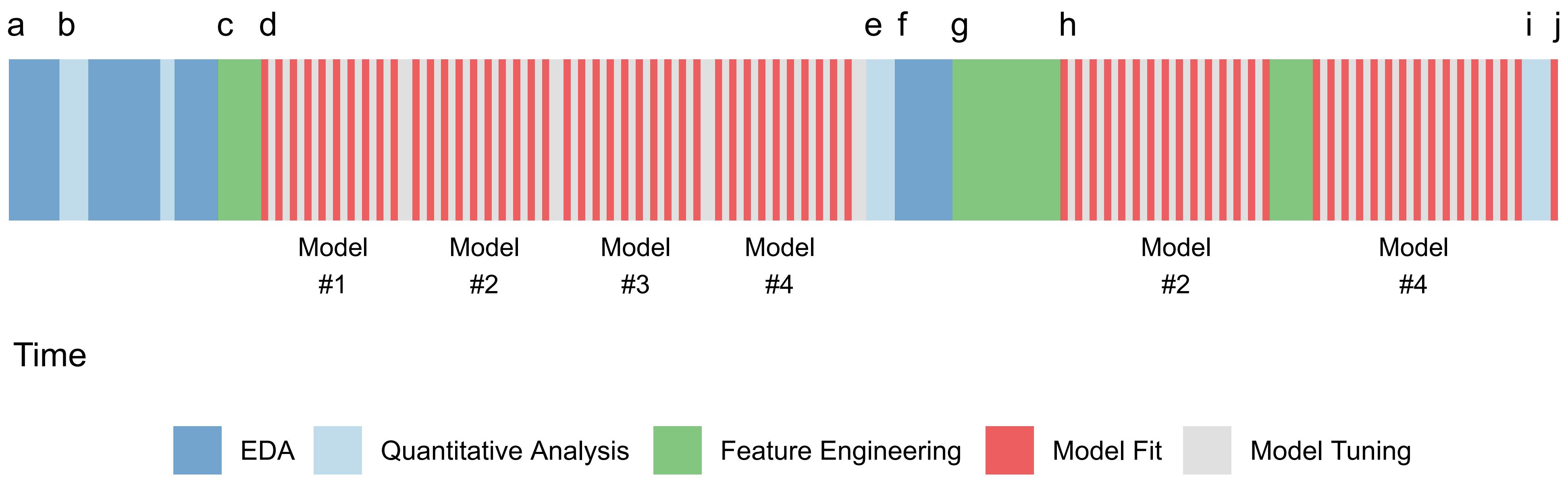
> We found coefficients by guess-and-check... is there a better way?

Practically: machine learning / stats software include efficient algorithms for exactly this. But it can still take weeks on supercomputers for big models and data.
Mathematically: Most common algorithm is *gradient descent*:

1. From your data, randomly pick a batch of a few observations.
2. Put those X's through your model, tracing the computations on the way.
3. Compute error (e.g., MSE) on that batch.
4. Compute *what small change to each coefficient would have reduced error*?
5. Make all of those small changes, repeat.

Objectives

- What are the basic steps in training and validating any predictive model?
- Why is each step important?
- How can we use the `tidymodels` ecosystem to train and validate a linear model?



Source: Feature Engineering and Selection ch1

Predictive Modeling Workflow

Preliminaries:

1. **Define the problem**: predict *what*, based on *what*? What *metrics* will indicate success? (Measure success in multiple ways!)
2. **Explore your data** (EDA): understand its structure, make lots of plots

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1. **Pick a model**: Which type(s) of models are appropriate for task and data?
2. **Transform the data** as needed by the model ("feature engineering", preprocessing", "recipe")
3. **Split the data** to allow for validation.
4. **Fit and evaluate the model**
5. **Tune**: adjust model hyperparameters
6. **Analyze model errors** and refine all earlier steps

```r
library(tidymodels)
```

Packages:

- `parsnip`: **Specify** and **train** the model you want
- `recipes`: **Prepare** the data
- `rsample`: **Split** data into training and validation
- `yardstick`: Compute **metrics** for performance
- `tune`: Helps you set the dials.

Analogous Python package: `scikit-learn`.

Where to find documentation

Theory

- Feature Engineering and Selection
- An Introduction to Statistical Learning

Practice

- TidyModels website: Getting Started, vignettes
- Tidy Modeling with R book (work in progress)

Some others:

- https://rviews.rstudio.com/2019/06/19/a-gentle-intro-to-tidymodels/
- https://juliasilge.com/blog/intro-tidymodels/

Example data: Ames home sales

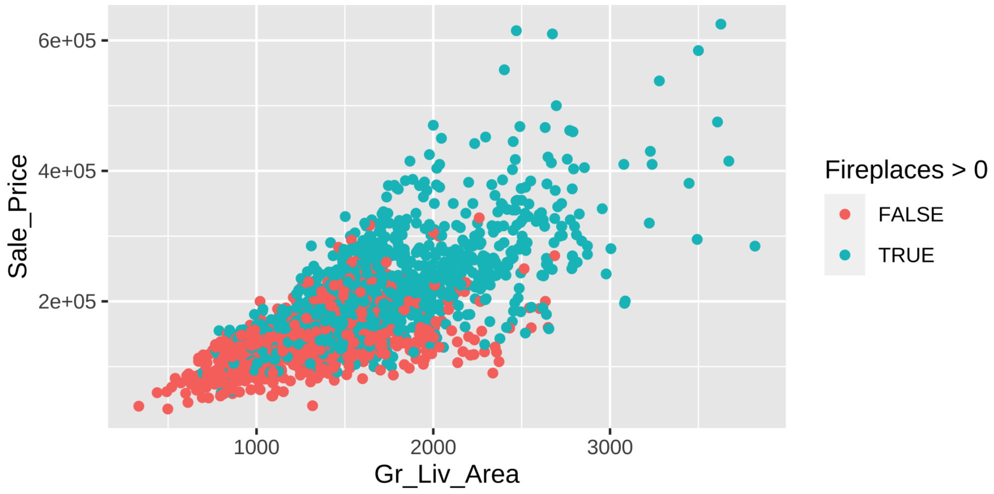
Like before, but we subset the data as De Cock suggests. Again, see Data dictionary

```
data(ames, package = "modeldata")
ames <- ames %>%
  filter(Gr_Liv_Area < 4000, Sale_Condition ==
nrow(ames)
```

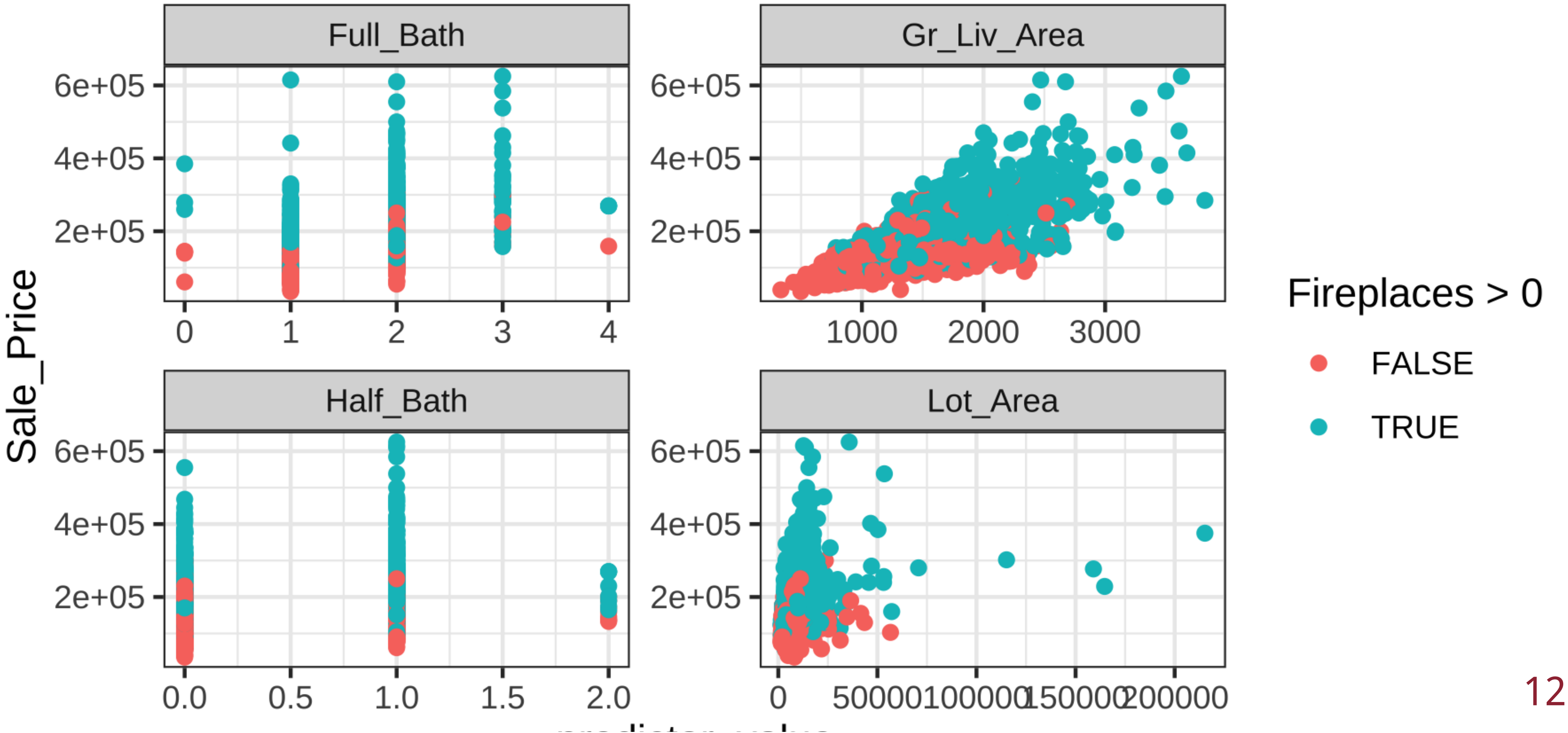
```
## [1] 2412
```

Exploratory analysis:

```
ggplot(ames, aes(x = Gr_Liv_Area, y = Sale_Pri
  geom_point()
```



```
ames %>% select(Sale_Price, Gr_Liv_Area, Lot_Area, Full_Bath, Half_Bath, Fireplaces) %>%
  pivot_longer(-c(Sale_Price, Fireplaces), names_to = "predictor", values_to = "predictor_value") %>
  ggplot(aes(x = predictor_value, y = Sale_Price, color = Fireplaces > 0)) + geom_point() +
  facet_wrap(vars(predictor), scales = "free") + theme_bw()
```



Example, without validation

Specify the model:

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my_model_spec <-  parsnip::linear_reg() %>%
  set_engine("lm")
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Predict on new data:

```
tibble(Lot_Area = c(32000, 12000), Sale_Price = c(239000, 185000)) %>%
  predict(my_trained_model, new_data = .)
```

```
## # A tibble: 2 x 1
##     .pred
##     <dbl>
## 1 226579.
## 2 179869.
```

Example, with validation

1. Hold out some data to use for validation:

```
set.seed(10)
ames_split <- initial_split(ames, prop = 3/4)
ames_train <- training(ames_split)
ames_test <- testing(ames_split)
glue("Using {nrow(ames_train)} sales to train, {nrow(ames_test)} to test")
```

```
## Using 1809 sales to train, 603 to test
```

1. Hold out some data to use for validation:
2. Specify the model to use.
3. Train the model **on the training set**:

```
my_trained_model <- my_model_spec %>%
  fit(Sale_Price ~ Lot_Area + Gr_Liv_Area + Full_Bath, data = ames_train)
```

1. Hold out some data to use for validation:
2. Specify the model to use.
3. Train the model **on the training set**
4. Make predictions on training set:

```
train_predictions <-
  my_trained_model %>%
    predict(ames_train)
train_predictions
```

```
## # A tibble: 1,809 x 1
##      .pred
##      <dbl>
## 1 115287.
## 2 156986.
## 3 200732.
## 4 194610.
## 5 210156.
## 6 199231.
## # … with 1,803 more rows
```

```
train_predictions %>%
  bind_cols(ames_train) %>% # Put back the orig
  yardstick::metrics(truth = Sale_Price, estima
```

```
## # A tibble: 3 x 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 rmse    standard   47334.
## 2 rsq     standard       0.557
## 3 mae     standard   31936.
```

1. Hold out some data to use for validation:
2. Specify the model to use.
3. Train the model **on the training set**
4. Make predictions on training set:
5. **Evaluate on test** set:

```
my_trained_model %>%
  predict(ames_test) %>%
  bind_cols(ames_test) %>%
  metrics(truth = Sale_Price, estimate = .pred)
```

```
## # A tibble: 3 x 3
##   .metric .estimator .estimate
##   <chr>   <chr>          <dbl>
## 1 rmse    standard   44606.
## 2 rsq     standard       0.548
## 3 mae     standard   32442.
```

Types of models

- Linear models
  - ordinary least-squares (OLS)
  - Lasso, Ridge, etc.: penalize large coefficients
  - Generalized Linear Models: outputs get transformed
  - Logistic Regression (also Support Vector Machine): transform output to *score* for each class
- Decision Lists and Trees
  - extension: Random Forests
- Neural Networks: layered combinations of the above
- many, many more

Which variables mean what?

The *formula interface*:

- `y ~ x`
  - predict *y* using *x*. `Sale_Price ~ Lot_Area`
- `y ~ x1 + x2 + x3`
  - predict *y* using *x1* and *x2* and *x3*
  - `Sale_Price ~ Lot_Area + Gr_Liv_Area + Full_Bath`

Don't get confused: they "forgot" the coefficients! A fitted linear model will actually look like:

Sale_Price = c1 * Lot_Area + c2 * Gr_Liv_Area + c3 * Full_Bath + intercept

But this works for specifying even models that aren't linear.