Chapter 3: Linear Regression

Linear regression is a simple approach for supervised learning when the response is quantitative. Linear regression has a long history and we could actually spend most of this semester talking about it.

Although linear regression is not the newest, shiniest thing out there, it is still a highly used technique out in the real world. It is also useful for talking about more modern techniques that are **generalizations** of it.

ridge regression, Lasso, Logistic regression, GAMs, etc.

We will review some key ideas underlying linear regression and discuss the <u>least squares</u> approach that is most commonly used to fit this model.

Linear regression can help us to answer the following questions about our Advertising data:

- 1. Is there a relationship both advertising and sales?
- 2. How strong is the relationship?
- 3. Which media contribute to sales?
- 4. How accurately can we spredict future sales?
- 5. How accurately can we estimate the effect of each medium on sales?
- 6. Is the relationship linear?
- 7. Is there synergy among the advertising media?
 i.e. is \$50K for TV and \$50kfor radio butter then \$100K m radio on TV alone?

Simple Linear Regression

Simple Linear Regression is an approach for prediction a quantitative response Y on the basis of a single predictor variable X.

It assumes:

Which leads to the following model:
$$Y = \beta_0 + \beta_1 \times + \mathcal{E}$$

For example, we may be interested in regressing sales onto TV by fitting the model

Sales = (Bo) + (B) x TV

Tintropt : slope unknown constats

"parameters" "model culfficients"

2 and 2 we can predict future

Once we have used training data to produce estimates $\hat{\beta}_0$ and $\hat{\beta}_1$, we can predict future sales on the basis of a particular TV advertising budget.

1.1 Estimating the Coefficients

In practice, β_0 and β_1 are **unknown**, so before we can predict \hat{y} , we must use our training data to estimate them.

1.1 Estimating the Coefficients

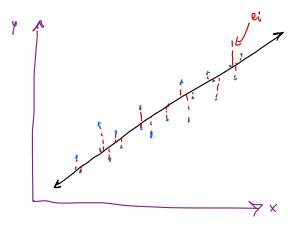
Let $(x_1, y_1), \ldots, (x_n, y_n)$ represent n observation pairs, each of which consists of a measurement of X and Y.

Goal: Obtain coefficient estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ such that the linear model fits the available data well.

We want to find on interrept fo and slope firs.t. The resulting line is dose to all a observations. The most common approach involves minimizing the least squares criterion.

Let
$$\hat{y_i} = \hat{\beta_0} + \hat{\beta_i} x_i$$
 prediction for γ based on its value of χ .
 $e_i = y_i - \hat{y}_i$ its residual

$$RSS = e_1^2 + ... + e_n^2$$
 residual sum of squares.



using calculus suffer boal for the derivatives, set = 0, solve for boal for the derivatives,

The least squares approach results in the following estimates:

$$\hat{\beta}_1 = \frac{\hat{z}_{i = 1}^2 (x_i - \bar{x})(y_i - \bar{y})}{\hat{z}_{i = 1}^2 (x_i - \bar{z})^{\frac{1}{2}}}$$

$$\hat{\beta}_0 = \bar{y}_0 - \hat{\beta}_1 \bar{x}$$
where $\hat{\beta}_0 = \bar{y}_0 - \hat{\beta}_1 \bar{x}$

beriensy ()

We can get these estimates using the following commands in R and tidymodels:

```
library(tidymodels) ## load library
         ## load the data in
         ads <- read_csv("../data/Advertising.csv", col_select = -1)</pre>
         ## fit the model
         lm spec <- linear reg() |>
           set mode("regression") |>
           set_engine("lm")
                           V least squares.
         slr fit <- lm spec |>
           fit(sales ~ TV, data = ads)
                                      Capecify data frame intraduly datan
                   YNX famile
                        "tegress Yorx"
         slr fit |>
          pluck("fit") |>
           summary()
The some as I'm (soles NTV, dota = ads) result of colly 1, "
         ## Call:
         ## stats::lm(formula = sales ~ TV, data = data)
         ## Residuals:
         ##
                 Min
                           1Q Median
                                             3Q
                                                    Max
         ## -8.3860 -1.9545 -0.1913
                                       2.0671
                                                7.2124
         ##
         ## Coefficients:
                         Estimate Std. Error t value Pr(>|t|)
                                                           <2e-16 ***
         ## (Intercept) 7.032594
                                      0.457843
                                                  15.36
         ## TV
                                                           <2e-16 ***
                          0.047537
                                      0.002691
                                                  17.67
         ## ---
         ## Signif. codes:
                              0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
         ## Residual standard error: 3.259 on 198 degrees of freedom
         ## Multiple R-squared: 0.6119, Adjusted R-squared: 0.6099
         ## F-statistic: 312.1 on 1 and 198 DF, p-value: < 2.2e-16
```

1.2 Assessing Accuracy

Recall we assume the *true* relationship between X and Y takes the form

If f is to be approximated by a linear function, we can write this relationship as average increase in Y associated
$$w/1$$
 unit inverse in X.

$$y = \beta_0 + \beta_1 \times + \varepsilon$$

Cotch-all for What we miss $w/1$ this simple model – the relationship may not be linear; may be often important variables not included; measure went error.

and when we fit the model to the training data, we get the following estimate of the population model

$$y = \hat{\beta}_0 + \hat{\beta}_1 \times$$

But how close this this to the truth? weasure w/ standard error

$$Ver(\hat{\beta}_0)^2 SE(\hat{\beta}_0)^2 = 6^2 \left[\frac{1}{n} + \frac{\overline{x}^2}{\Sigma_{i=1}^2(x_i - \overline{x})^2} \right]$$

$$Ver(\hat{\beta}_i) = SE(\hat{\beta}_i)^2 = 6^2 \left[\frac{1}{\sum_{i=1}^n (x_i - \overline{x}_i)^2} \right]$$

In general, $\underbrace{\sigma^2}_{\text{is not known}}$, so we estimate it with the residual standard error,

We can use these standard errors to compute confidence intervals and perform hypothesis tests.

95% CI for
$$\beta_0$$
: $\hat{\beta}_0 \pm \lambda SE(\hat{\beta}_0)$.

$$t = \frac{\beta_1 - 0}{SE(\beta_1^2)} \sim t_{\eta-2} \implies \text{compute } p(\text{observing ang number again to or more extreme than } |t|) = p-value \\ \text{Small } p\text{-value means highly unlikely to see this } t \text{ given tho} \\ \Rightarrow \text{reject } Ho$$

slr fit |>

Once we have decided that there is a significant linear relationship between X and Y that is captured by our model, it is natural to ask

To what extent does the model fit the data?

The quality of the fit is usually measured by the *residual standard error* and the \mathbb{R}^2 statistic.

RSE: Roughly speaking, the RSE is the average amount that the response will deviate from the true regression line. This is considered a measure of the *lack of fit* of the model to the data.

 R^2 : The RSE provides an absolute measure of lack of fit, but is measured in the units of Y. So, we don't know what a "good" RSE value is! R^2 gives the proportion of variation in Y explained by the model.

```
pluck("fit") |>
  summary()
##
## Call:
   stats::lm(formula = sales ~ TV, data = data)
## Residuals:
##
       Min
                 1Q Median
                                  3Q
                                         Max
  -8.3860 -1.9545 -0.1913
                            2.0671
                                      7.2124
                                              Ho: Pi=0 vs. Ha: Ri =0 i=0,1.
                          SE(B), SE(B))
   Coefficients:
##
               Estimate Std. Error t value Pr(>|t|)
  (Intercept)
                7.032594
                           0.457843
                                       15.36
                                               <2e-16 ***
                                       17.67
## TV
                0.047537
                           0.002691
                                               <2e-16 ***
                     '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '
## Signif. codes:
##
## Residual standard error: 3.259 on 198 degrees of freedom
## Multiple R-squared: (0.6119) Adjusted R-squared: 0.6099 ren's later
## F-statistic: 312.1 on 1 and 198 DF, p-value: < 2.2e-16
```

R2 = proportion of variability in y
explained by a linear relationship or/ X

2 Multiple Linear Regression

Simple linear regression is useful for predicting a response based on one predictor variable, but we often have **more than one** predictor.

How can we extend our approach to accommodate additional predictors?

We interpret β_j^{ψ} as the "average effect on Y of a one unit increase in X_j , holding all other predictors fixed".

In our Advertising example,

2.1 Estimating the Coefficients

As with the case of simple linear regression, the coefficients $\beta_0, \beta_1, \ldots, \beta_p$ are unknown and must be estimated. Given estimates $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p$, we can make predictions using the formula

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 \times_1 + ... + \hat{\beta}_p x_p.$$

The parameters are again estimated using the same <u>least squares approach</u> that we saw in the context of simple linear regression.

mlr_fit <- lm_spec |> fit(sales ~ TV + radio + newspaper, data = ads) mlr_fit <- lm_spec |> ~ linear wold specification from before. fit(sales ~ (), data = ads) Formula y w every other column in data frame. mlr fit |> pluck("fit") |> summary() ## ## stats::lm(formula = sales ~ ., data = data) ## ## Residuals: Min 1Q Median Max ## -8.8277 -0.8908 0.2418 1.1893 2.8292 ## Coefficients: ## Estimate Std. Error t value Pr(>|t|) 2.938889 B 0.311908 9.422 ## (Intercept) ## TV 32.809 <2e-16 *** 0.188530 0.008611 ## radio 21.893 <2e-16 *** -0.001037 B 0.005871 ## newspaper -0.1770.86 ## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 ## Residual standard error: 1.686 on 196 degrees of freedom ## Multiple R-squared: 0.8972, Adjusted R-squared: 0.8956

F-statistic: 570.3 on 3 and 196 DF, p-value: < 2.2e-16

now instead of now instead of a live, we are planted a hyperplanted a hyperplanted as a live of the north of

2.2 Some Important Questions

When we perform multiple linear regression we are usually interested in answering a few important questions:

- 1. Is at least one of the predictors X1, xp useful in predicting the response?
- 2. Do all predictors help explain Y, or only asubut is usefue?
- 3. It on well does model fit data?
- 4. briun a set of predictors values what response should me predict and how accurate is our prediction?

2.2.1 Is there a relationship between response and predictors?

We need to ask whether <u>all</u> of the regression coefficients are zero, which leads to the following hypothesis test.

$$H_0: \beta_1 = \beta_2 = \dots = \beta_p = 0$$

$$H_a$$
: at least me β_j is non-zero.

This hypothesis test is performed by computing the F-statistic

Variance in response explained by
$$F = \frac{(TSS - RSS)/p}{RSS/(n-p-1)}$$
 $V_p, n-p-1$ $V_p, n-p-1$

2.2.2 Deciding on Important Variables

After we have computed the F-statistic and concluded that there is a relationship between predictor and response, it is natural to wonder

Which predictors are related to the response?

We could look at the p-values on the individual coefficients, but if we have many variables this can lead to false discoveries.

Instead we could consider variable selection. We will revisit this in Ch. 6.

2.2.3 Model Fit

Two of the most common measures of model fit are the RSE and R^2 . These quantities are computed and interpreted in the same way as for simple linear regression.

Be careful with using these alone, because R^2 will **always increase** as more variables are added to the model, even if it's just a small increase.

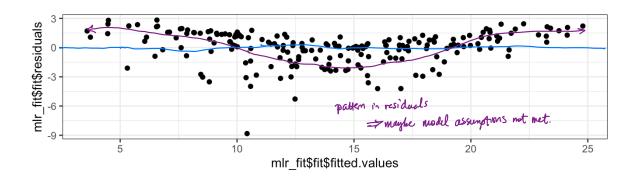
```
How to avoid overfitting?
Use test data! Chu5
# model with TV, radio, and newspaper
mlr fit |> pluck("fit") |> summary()
##
## Call:
## stats::lm(formula = sales ~ ., data = data)
                                                           individual slopes hypothesis test

Ho: Bj=0 j=0,..,p

Ha: Bj =0
## Residuals:
       Min
                 1Q Median
                                   3Q
                                           Max
## -8.8277 -0.8908
                      0.2418
                              1.1893
                                        2.8292
##
## Coefficients:
                 Estimate Std. Error t value Pr(>|t|)
                 2.938889
                              0.311908
                                          9.422
                                                   <2e-16 ***
## (Intercept)
## TV
                 0.045765
                              0.001395
                                         32.809
                                                   <2e-16 ***
                 0.188530
                              0.008611
                                         21.893
                                                   <2e-16 ***
## radio
                -0.001037
                              0.005871
                                         -0.177
                                                     0.86
## newspaper
                     0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Signif. codes:
## Residual standard error: 1.686 on 196 degrees of freedom
## Multiple R-squared: 0.8972, Adjusted R-squared: 0.8956
## F-statistic: 570.3 on 3 and 196 DF, p-value: < 2.2e-16
```

```
# model without newspaper
 lm_spec |> fit(sales ~ TV + radio, data = ads) |>
   pluck("fit") |> summary()
 ##
 ## Call:
 ## stats::lm(formula = sales ~ TV + radio, data = data)
 ##
 ## Residuals:
 ##
        Min
                 1Q Median
                                  30
                                         Max
 ## -8.7977 -0.8752 0.2422 1.1708 2.8328
 ## Coefficients:
                Estimate Std. Error t value Pr(>|t|)
 ## (Intercept) 2.92110 0.29449
                                      9.919
                                               <2e-16 ***
 ## TV
                 0.04575
                             0.00139 32.909
                                                <2e-16 ***
 ## radio
                 0.18799
                             0.00804 23.382
                                                <2e-16 ***
                     0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
 ## Signif. codes:
 ## Residual standard error: 1.681 on 197 degrees of freedom
 ## Multiple R-squared: (0.8972, Adjusted R-squared: 0.8962
 ## F-statistic: 859.6 on 2 and 197 DF, p-value: < 2.2e-16
                                 R2 barely decreased when we took out pewspaper
It may also be useful to plot residuals to get a sense of the model fit.
                         ei = y:- ŷi
```

ggplot() +
 geom_point(aes(mlr_fit\$fit\$fitted.values, mlr_fit\$fit\$residuals))



Want: random noise around zero, no payen.

3 Other Considerations

3.1 Categorical Predictors

So far we have assumed all variables in our linear model are quantitiative.

what to do when X; cotyonial?

For example, consider building a model to predict highway gas mileage from the mpg data set.

head(mpg)

```
## # A tibble: 6 × 11
     manufacturer model displ year
                                        cyl trans
                                                        drv
                                                                cty
                                                                       hwy
fl
      class
                  <chr> <dbl> <int> <int> <chr>
                                                        <chr> <int> <int>
##
     <chr>
<chr> <chr>
## 1 audi
                  a4
                           1.8
                                1999
                                          4 auto(15)
                                                        f
                                                                 18
                                                                        29
      compa...
## 2 audi
                  a4
                           1.8
                                1999
                                          4 manual(m5) f
                                                                 21
                                                                        29
      compa...
                                      4 manual(m6) f
## 3 audi
                                2008
                                                                 20
                                                                        31
                  a4
      compa...
## 4 audi
                  a4
                                2008
                                          4 auto(av)
                                                                        30
      compa...
## 5 audi
                                          6 auto(15)
                           2.8
                                1999
                                                                        26
                                                        f
      compa...
## 6 audi
                   a4
                           2.8 1999
                                          6 manual(m5) f
                                                                 18
                                                                        26
      compa...
```

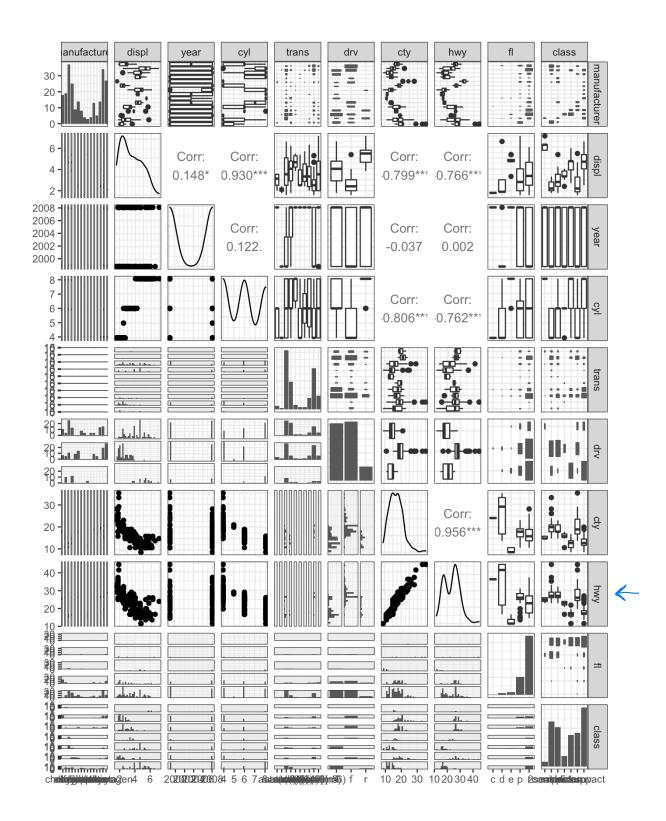
```
library(GGally)
```

```
mpg %>%

select(-model) %>% # too many models

ggpairs() # plot matrix

[makes p(p-1) plots to look I each pair of variables h data frame.
```



To incorporate these categorical variables into the model, we will need to introduce k-1 dummy variables, where k = the number of levels in the variable, for each qualitative variable.

```
For example, for dry, we have 3 levels: 4, f, and r.
 lm spec |>
   fit(hwy ~ displ + cty + drv, data = mpg) |>
   pluck("fit") |>
                        Categorical variable
   summary()
 ##
 ## Call:
 ## stats::lm(formula = hwy ~ displ + cty + drv, data = data)
 ##
 ## Residuals:
       Min
               1Q Median
                            3Q
                                  Max
 ## -4.6499 -0.8764 -0.3001 0.9288 4.8632
 ##
 ## Coefficients:
             Estimate Std. Error t value Pr(>|t|)
                               3.132 0.00196 **
 ## (Intercept) 3.42413 1.09313
             -0.20803 0.14439 -1.441 0.15100
 ## displ
              1.15717 0.04213 27.466 < 2e-16 ***
 ## cty
             → ## drvf
>## drvr
             2.35970 0.37013 6.375 9.95e-10 ***
 ## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
 ##
 ## Residual standard error: 1.49 on 229 degrees of freedom
 ## Multiple R-squared: 0.9384, Adjusted R-squared: 0.9374
 ## F-statistic: 872.7 on 4 and 229 DF, p-value: < 2.2e-16
```

3.2 Extensions of the Model

The standard regression model provides interpretable results and works well in many problems. However it makes some very strong assumptions that may not always be reasonable.

& linear relationship constat error variance uncorrelated errors w/X

Additive Assumption

The additive assumption assumes that the effect of each predictor on the response is not affected by the value of the other predictors. What if we think the effect should depend on the value of another predictor?

```
lm spec |>
  fit(sales ~ TV + radio + (TV*radio), data = ads) |>
  pluck("fit") |>
                            y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \varepsilon
  summary()
                               = \beta_0 + (\beta_1 + \beta_3 X_2) X_1 + \beta_2 X_2 + \epsilon
##
                               = Bo + BIX1+ (B2+ BOX1) X2 +E
## Call:
## stats::lm(formula = sales ~ TV + radio + TV * radio, data = data)
##
## Residuals:
##
        Min
                   10 Median
                                              Max
## -6.3366 -0.4028
                       0.1831
                                0.5948
                                          1.5246
##
## Coefficients:
##
                  Estimate Std. Error t value Pr(>|t|)
## (Intercept) 6.750e+00 2.479e-01 27.233
                                                    <2e-16 ***
                                                      <2e-16 *** $\beta_3$ significantly differ from 0.
## TV
                 1.910e-02 1.504e-03
                                          12.699
## radio
                  2.886e-02 8.905e-03
                                           3.241
## TV:radio
                 1.086e-03 5.242e-05 20.727
                      0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## Signif. codes:
##
## Residual standard error: 0.9435 on 196 degrees of freedom
## Multiple R-squared: 0.9678, Adjusted R-squared: 0.9673
## F-statistic: 1963 on 3 and 196 DF, p-value: < 2.2e-16 _ significant relativistic
                               R<sup>2</sup> = ,89 inflood interaction
big increase >> butter-fitting model.
```

" an increase of \$1000 in tadio advertising will be associated u/ an expected therease it sales of (\$2+B3*TV) × 1000 = 29+1.1 TV"

* If we include interaction term be sure to keep the original variables, otherwise interpretation is confusing.

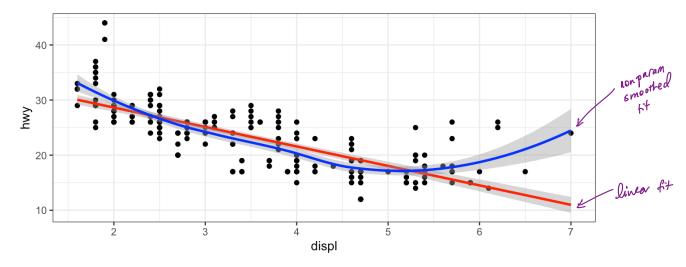
```
" recipe" is plan to fit model.
Alternatively:
 rec_spec_interact <- recipe(sales ~ TV + radio, data = ads) |>

→ step_interact(~ TV:radio)
 lm_wf_interact <- workflow() |>
    add_model(lm_spec) |>
    add_recipe(rec_spec_interact)
  lm wf interact |> fit(ads)
  ## == Workflow [trained]
 ## Preprocessor: Recipe
 ## Model: linear_reg()
 ##
  ## — Preprocessor
 ## 1 Recipe Step
 ##
 ## • step_interact()
  ##
  ## - Model
  ##
 ## Call:
 ## stats::lm(formula = ..y ~ ., data = data)
  ## Coefficients:
 ## (Intercept)
                           TV
                                      radio
                                              TV x radio
  ##
        6.750220
                   0.019101
                                 0.028860
                                                0.001086
```

Linearity Assumption

The linear regression model assumes a linear relationship between response and predictors. In some cases, the true relationship may be non-linear.

```
ggplot(data = mpg, aes(displ, hwy)) +
  geom_point() +
  geom_smooth(method = "lm", colour = "red") +
  geom_smooth(method = "loess", colour = "blue")
```



How to include non-linear terms in the most?

```
"Identity"
 lm_spec |>
   fit(hwy ~ displ + (1(displ^2), data = mpg) |>
   pluck("fit") |> summary()
 ##
 ## Call:
 ## stats::lm(formula = hwy ~ displ + I(displ^2), data = data)
 ## Residuals:
       Min
                1Q Median
                                 30
                                        Max
 ## -6.6258 -2.1700 -0.7099 2.1768 13.1449
 ## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
 ## ---
 ## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
 ## Residual standard error: 3.423 on 231 degrees of freedom
 ## Multiple R-squared: 0.6725, Adjusted R-squared: 0.6696
 ## F-statistic: 237.1 on 2 and 231 DF, p-value: < 2.2e-16
 Be coreful throwing higher order terms -> can lead the objectiving is very bad predictions on edges of the space.

Uill some back to a letter way to do this later.
3.3 Potential Problems
```

- 1. Non-linearity of response-predictor relationships
- 2. Correlation of error terms
- 3. Non-constant variance of error terms
- 4. Outliers

4 K-Nearest Neighbors

In Ch. 2 we discuss the differences between *parametric* and *nonparametric* methods. Linear regression is a parametric method because it assumes a linear functional form for f(X).

A simple and well-known non-parametric method for regression is called K-nearest neighbors regression (KNN regression).

Given a value for K and a prediction point x_0 , KNN regression first identifies the K training observations that are closest to x_0 (\mathcal{N}_0). It then estimates $f(x_0)$ using the average of all the training responses in \mathcal{N}_0 ,

```
set.seed(445) #reproducibility
## generate data
x <- rnorm(100, 4, 1) # pick some x values
y < -0.5 + x + 2*x^2 + rnorm(100, 0, 2) # true relationship
df \leftarrow data.frame(x = x, y = y) # data frame of training data
for (k in seq(2, 10, by = 2)) {
  nearest neighbor(mode = "regression", neighbors = k) |>
    fit(y \sim x, data = df) >
    augment(new data = df) |>
    ggplot() +
    geom\ point(aes(x, y)) +
    geom_line(aes(x, .pred), colour = "red") +
    ggtitle(paste("KNN, k = ", k)) +
    theme(text = element text(size = 30)) -> p
 print(p)
}
lm spec |>
  fit(y \sim x, df) >
  augment(new_data = df) |>
  ggplot() +
    geom\ point(aes(x, y)) +
    geom line(aes(x, .pred), colour = "red") +
```

```
ggtitle("Simple Linear Regression") +
theme(text = element_text(size = 30)) # slr plot
```

