

# 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 least squares 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 btw/ advertising and sales?*
2. *How strong is the relationship?*
3. *Which media contribute to sales?*
4. *How accurately can we predict 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 \$50K for radio better than \$100K on radio or TV alone?*

# 1 Simple Linear Regression

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

It assumes:

- approximately linear relationship between  $X$  and  $Y$
- random error term has constant variance
- random error term is Normally distributed.

Which leads to the following model:

$$Y = \beta_0 + \beta_1 X + \varepsilon$$

*Linear relationship*

$$\varepsilon \sim N(0, \sigma^2)$$

*assumptions about error*

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

$$\text{sales} = \beta_0 + \beta_1 \times \text{TV}$$

*intercept* *slope* *unknown constants*  
*"parameters"* *"model coefficients"*

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.

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

*prediction of sales* *particular TV budget value*

## 1.1 Estimating the Coefficients

In practice,  $\beta_0$  and  $\beta_1$  are **unknown**, so before we can predict  $\hat{y}$ , we must use our training data to estimate them.

*"fit the model"*

### Training data

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

In the advertising data,

$X$  = TV ad budget

$Y$  = sales

$n = 200$  markets.

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

i.e.  $y_i \approx \hat{\beta}_0 + \hat{\beta}_1 x_i$  for  $i = 1, \dots, n$

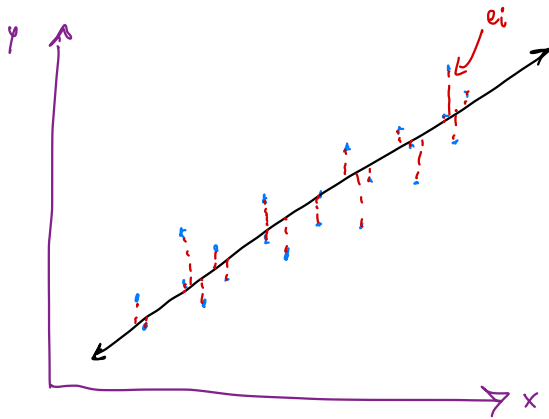
We want to find an intercept  $\hat{\beta}_0$  and slope  $\hat{\beta}_1$  s.t. the resulting line is "close" to all  $n$  observations. The most common approach involves minimizing the *least squares* criterion.

Let  $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$  prediction for  $Y$  based on  $i^{\text{th}}$  value of  $X$ .

$e_i = y_i - \hat{y}_i$   $i^{\text{th}}$  residual

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

choose  $\hat{\beta}_0$  and  $\hat{\beta}_1$  to minimize  $RSS$ .



using calculus  
take derivatives, set = 0, solve for  $\hat{\beta}_0$  and  $\hat{\beta}_1$

The least squares approach results in the following estimates:

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

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

"least squares  
coefficients"

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)

## fit the model
lm_spec <- linear_reg() |>
  set_mode("regression") |>
  set_engine("lm")

slr_fit <- lm_spec |>
  fit(sales ~ TV, data = ads)

slr_fit |>
  pluck("fit") |>
  summary()
```

*Handwritten notes:*

- previously used lm()*
- Model specification*
- least squares*
- Y ~ X formula*
- specify data frame*
- regress Y on X*
- training data*
- exactly the same as result of calling lm(sales ~ TV, data = ads)*

```
##
## 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|)
## (Intercept)  7.032594   0.457843   15.36  <2e-16 ***
## TV           0.047537   0.002691   17.67  <2e-16 ***
## ---
## 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
```

*Handwritten notes:*

- $\hat{\beta}_0$
- $\hat{\beta}_1$

## 1.2 Assessing Accuracy

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

$$Y = f(X) + \varepsilon, \quad f \text{ is unknown, } \varepsilon \text{ mean-zero random error.}$$

If  $f$  is to be approximated by a linear function, we can write this relationship as

$$Y = \beta_0 + \beta_1 X + \varepsilon$$

population regression line.

average increase in  $Y$  associated w/ 1 unit increase in  $X$ .

catch-all for what we miss w/ this simple model - true relationship may not be linear; may be other important variables not included; measurement error.

expected value of  $Y$  when  $X=0$

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

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X$$

least squares line.

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

$$\text{Var}(\hat{\beta}_0) = \text{SE}(\hat{\beta}_0)^2 = \sigma^2 \left[ \frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right]$$

$$\text{Var}(\hat{\beta}_1) = \text{SE}(\hat{\beta}_1)^2 = \sigma^2 \left[ \frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2} \right]$$

In general,  $\sigma^2$  is not known, so we estimate it with the *residual standard error*,  
 $RSE = \sqrt{RSS/(n-2)}$ .

residual sum of squares

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

$$95\% \text{ CI for } \beta_1: \hat{\beta}_1 \pm 2 \text{SE}(\hat{\beta}_1)$$

$$95\% \text{ CI for } \beta_0: \hat{\beta}_0 \pm 2 \text{SE}(\hat{\beta}_0).$$

approx normality of  $\hat{\beta}_1$

Hypothesis tests:

$$H_0: \text{There is no relationship btw/ } X \text{ and } Y \iff H_0: \beta_1 = 0$$

$$H_a: \text{There is a relationship btw/ } X \text{ and } Y \iff H_a: \beta_1 \neq 0$$

? : is  $\hat{\beta}_1$  far enough away from 0 to be confident it is nonzero?

$$t = \frac{\hat{\beta}_1 - 0}{\text{SE}(\hat{\beta}_1)} \sim t_{n-2} \Rightarrow \text{compute } p(\text{observing any number equal to or more extreme than } |t|) = p\text{-value}$$

(under  $H_0$ )

Small p-value means highly unlikely to see this  $t$  given  $H_0$

$\Rightarrow$  reject  $H_0$

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  $R^2$  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. *i.e. will always be between 0 and 1.*

*Advertising data example.*

```
slr_fit |>
  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
##
## Coefficients:  $\hat{\beta}_0, \hat{\beta}_1$   $SE(\hat{\beta}_0), SE(\hat{\beta}_1)$   $H_0: \beta_i = 0$  vs.  $H_a: \beta_i \neq 0$   $i=0,1$ 
##      Estimate Std. Error t value Pr(>|t|)
## (Intercept)  7.032594   0.457843   15.36 <2e-16 ***
## TV          0.047537   0.002691   17.67 <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3.259 A.R.E on 198 degrees of freedom
## Multiple R-squared: 0.6119, Adjusted R-squared: 0.6099 review later.
## F-statistic: 312.1 on 1 and 198 DF, p-value: < 2.2e-16
```

$R^2$  = proportion of variability in  $Y$   
explained by a linear relationship w/  $X$

## 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 could run separate SLR for each predictor

But! How to make a single prediction for  $Y$  based on levels of all predictors?

Also each model would ignore the other predictors ... what if they are related?

→ misleading results.

Solution: We can give each predictor a separate slope coefficient in a single model.

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + \varepsilon$$

We interpret  $\beta_j^{\downarrow}$  as the “average effect on  $Y$  of a one unit increase in  $X_j$ , holding all other predictors fixed”.

In our Advertising example,

$$\text{Sales} = \beta_0 + \beta_1 \text{TV} + \beta_2 \text{radio} + \beta_3 \text{newspaper} + \varepsilon$$

## 2.1 Estimating the Coefficients

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

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \dots + \hat{\beta}_p x_p.$$

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

*now instead of a line, we are fitting a hyperplane.*

```
# mlr_fit <- lm_spec /> fit(sales ~ TV + radio + newspaper, data = ads)
mlr_fit <- lm_spec |> ← linear model specification from before.
  fit(sales ~ •, data = ads)
    formula y ~ every other column in data frame.

mlr_fit |>
→ pluck("fit") |>
  summary()
```

*alternatively*

*pull out fit object*

```
##
## Call:
## stats::lm(formula = sales ~ ., data = data)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -8.8277 -0.8908  0.2418  1.1893  2.8292
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  2.938889 β̂₀ 0.311908   9.422  <2e-16 ***
## TV           0.045765 β̂₁ 0.001395  32.809  <2e-16 ***
## radio        0.188530 β̂₂ 0.008611  21.893  <2e-16 ***
## newspaper   -0.001037 β̂₃ 0.005871  -0.177    0.86
## ---
## 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
```



## 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  $X_1, \dots, X_p$  useful in predicting the response?
2. Do all predictors help explain  $Y$ , or only a subset is useful?
3. How well does model fit data?
4. Given a set of predictors values what response should we predict and how accurate is our prediction?

### 2.2.1 Is there a relationship between response and predictors?

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

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

$$H_a : \text{at least one } \beta_j \text{ is non-zero.}$$

This hypothesis test is performed by computing the  $F$ -statistic

$$F = \frac{\text{variance in response explained by model} \quad (TSS - RSS)/p}{\text{variance unexplained by model} \quad RSS/(n-p-1)} \sim F_{p, n-p-1} \text{ under } H_0$$

if this ratio  $F$  is large (much larger than 1), evidence against the null  $H_0$ , i.e. evidence there is some relationship.

### 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.

forward selection,  
backward selection,  
\* Lasso \*

### 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! Ch. 5

```
# model with TV, radio, and newspaper
mlr_fit |> pluck("fit") |> summary()
```

```
##
## Call:
## stats::lm(formula = sales ~ ., data = data)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -8.8277 -0.8908  0.2418  1.1893  2.8292
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  2.938889   0.311908   9.422  <2e-16 ***
## TV           0.045765   0.001395  32.809  <2e-16 ***
## radio        0.188530   0.008611  21.893  <2e-16 ***
## newspaper   -0.001037   0.005871  -0.177    0.86
## ---
## 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
```

individual slopes hypothesis test  
 $H_0: \beta_j = 0$   
 $H_a: \beta_j \neq 0$   $j = 0, \dots, p$

$R^2$  → 89.72% of variability in  $y$  is captured by this linear model.

F-test

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

$H_a: \beta_j \neq 0 \quad j \in \{1, \dots, p\}$

$F \sim F_{3, 196}$   
under  $H_0$

prob of seeing F stat value as or more extreme than 570.3 if  $H_0$  true.

```
# model without newspaper
lm_spec |> fit(sales ~ TV + radio, data = ads) |>
  pluck("fit") |> summary()

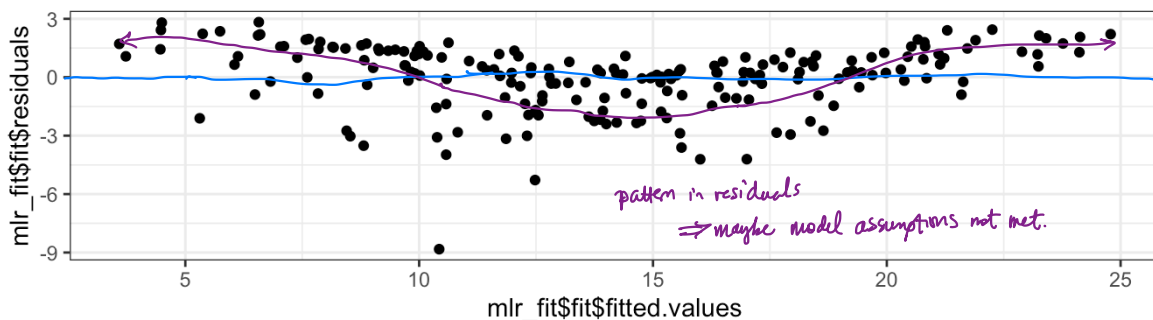
##
## Call:
## stats::lm(formula = sales ~ TV + radio, data = data)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -8.7977 -0.8752  0.2422  1.1708  2.8328
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)   2.92110    0.29449   9.919  <2e-16 ***
## TV            0.04575    0.00139  32.909  <2e-16 ***
## radio         0.18799    0.00804  23.382  <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## 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
```

$R^2$  barely decreased when we took out newspaper  $\Rightarrow$  not contributing much.

It may also be useful to plot residuals to get a sense of the model fit.

$$e_i = y_i - \hat{y}_i$$

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



Want: random noise around zero, no pattern.

QQ plot  
residuals vs. each predictor

## 3 Other Considerations

### 3.1 Categorical Predictors

So far we have assumed all <sup>predictor + response</sup> variables in our linear model are quantitative. <sup>what to do when  $X_i$  categorical?</sup>

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

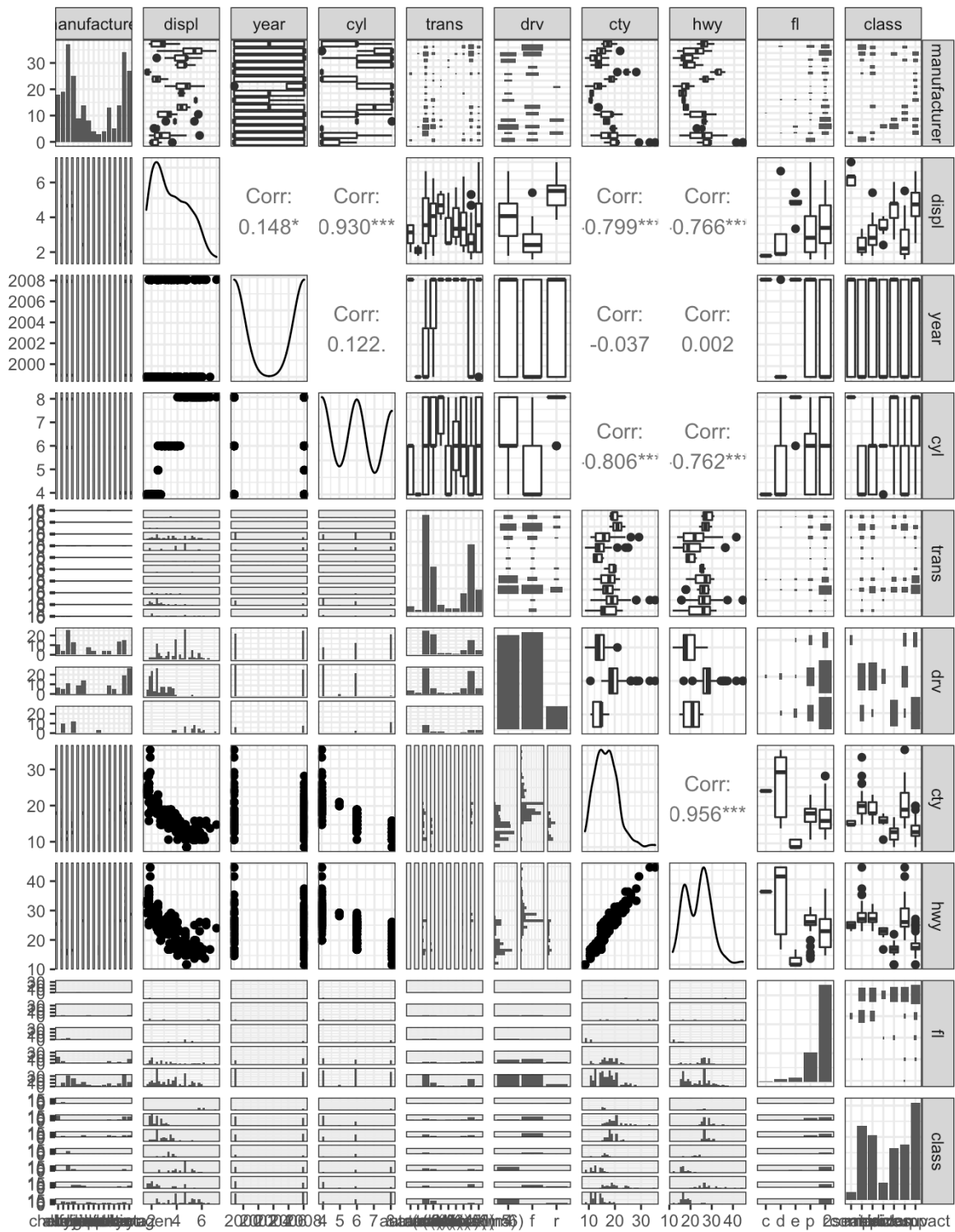
```
head(mpg)
```

```
## # A tibble: 6 × 11
##   manufacturer model displ  year   cyl trans      drv    cty   hwy
##   <chr>          <chr> <dbl> <int> <int> <chr>    <chr> <int> <int>
##   <chr> <chr>
## 1 audi          a4      1.8  1999     4 auto(l5)  f      18    29
p    compa...
## 2 audi          a4      1.8  1999     4 manual(m5) f      21    29
p    compa...
## 3 audi          a4      2    2008     4 manual(m6) f      20    31
p    compa...
## 4 audi          a4      2    2008     4 auto(av)   f      21    30
p    compa...
## 5 audi          a4      2.8  1999     6 auto(l5)  f      16    26
p    compa...
## 6 audi          a4      2.8  1999     6 manual(m5) f      18    26
p    compa...
```

```
library(GGally)
```

```
mpg %>%
  select(-model) %>% # too many models
  ggpairs() # plot matrix
```

↑ makes  $\frac{p(p-1)}{2}$  plots to look at each pair of variables in 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 `drv`, we have 3 levels: 4, f, and r. ↖  $k=3$

$$x_{i1} = \begin{cases} 1 & \text{if the car is FWD} \\ 0 & \text{if the car is not FWD} \end{cases}$$

$$x_{i2} = \begin{cases} 1 & \text{if the car is RWD} \\ 0 & \text{if the car is not RWD} \end{cases}$$

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \varepsilon_i = \begin{cases} \beta_0 + \beta_1 + \varepsilon_i & \text{if the car is FWD} \\ \beta_0 + \beta_2 + \varepsilon_i & \text{if the car is RWD} \\ \beta_0 + \varepsilon_i & \text{if the car is 4WD} \end{cases}$$

$\beta_0 =$  avg hwy mpg for 4WD cars

$\beta_1 =$  difference in average hwy btw/ FWD and 4WD cars.

$\beta_2 =$  difference in average hwy btw/ RWD and 4WD cars.

```
lm_spec |>
  fit(hwy ~ displ + cty + drv, data = mpg) |>
  pluck("fit") |>
  summary()
```

↑ quantitative variables.

↑ categorical variable

```
##
## 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|)
## (Intercept)   3.42413    1.09313   3.132  0.00196 **
## displ        -0.20803    0.14439  -1.441  0.15100
## cty           1.15717    0.04213  27.466 < 2e-16 ***
## drv[f]        2.15785    0.27348   7.890 1.23e-13 ***
## drv[r]        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  
constant 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") |>
  summary()
```

interaction term.

$$\begin{aligned}
 Y &= \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 + \varepsilon \\
 &= \beta_0 + (\beta_1 + \beta_3 X_2) X_1 + \beta_2 X_2 + \varepsilon \\
 &= \beta_0 + \beta_1 X_1 + (\beta_2 + \beta_3 X_1) X_2 + \varepsilon
 \end{aligned}$$

```
##
## Call:
## stats::lm(formula = sales ~ TV + radio + TV * radio, data = data)
##
## Residuals:
##      Min       1Q   Median       3Q      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 ***
## TV           1.910e-02  1.504e-03  12.699  <2e-16 ***
## radio        2.886e-02  8.905e-03   3.241  0.0014 **
## TV:radio      1.086e-03  5.242e-05  20.727  <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## 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
```

β<sub>3</sub> significantly different from 0.

R<sup>2</sup> = 0.89 without interaction  
big increase ⇒ better-fitting model.

significant relationship

"an increase of \$1000 in radio advertising will be associated w/ an expected increase in sales of  $(\hat{\beta}_2 + \hat{\beta}_3 \times TV) \times 1000 = 29 + 1.1 TV$ "

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

Alternatively:

"recipe" → plan the fit model.

interaction step  
transformation of  
matrix X

```
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
```

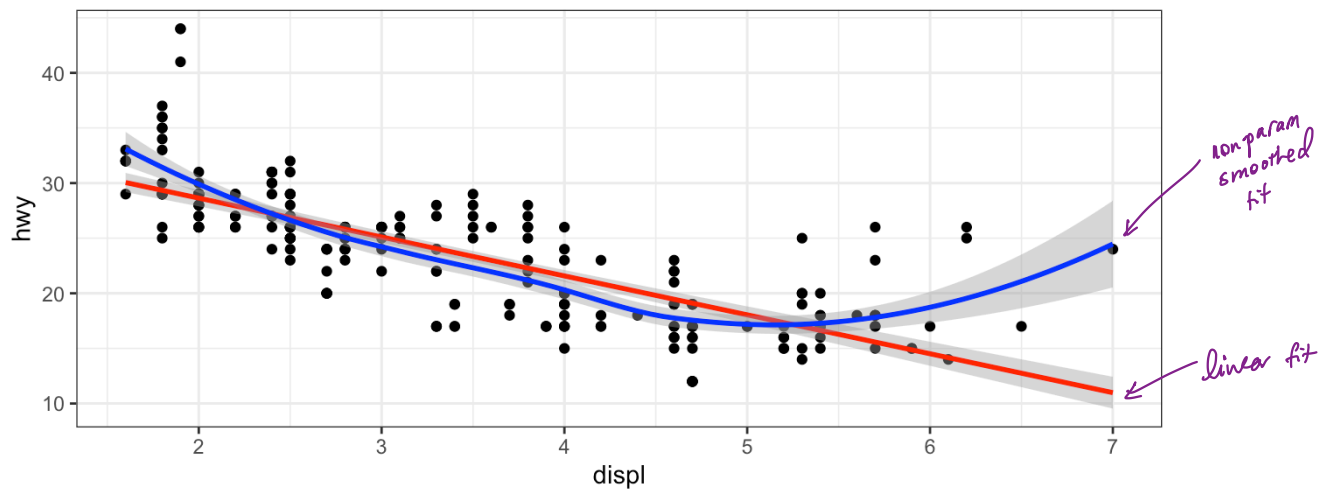
```
##
## Call:
## stats::lm(formula = ..y ~ ., data = data)
##
## Coefficients:
## (Intercept)          TV          radio    TV_x_radio
##    6.750220    0.019101    0.028860    0.001086
```



## 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 model?*

```

lm_spec |>
  fit(hwy ~ displ + I(displ^2), data = mpg) |>
  pluck("fit") |> summary()

```

"Identity"

```

##
## Call:
## stats::lm(formula = hwy ~ displ + I(displ^2), data = data)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -6.6258 -2.1700 -0.7099  2.1768 13.1449
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)   49.2450     1.8576  26.510 < 2e-16 ***
## displ        -11.7602     1.0729 -10.961 < 2e-16 ***
## I(displ^2)     1.0954     0.1409   7.773 2.51e-13 ***
## ---
## 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

```

Significant.

Be careful throwing higher order terms → can lead to overfitting? very bad predictions on edges of the space.  
 Will come back to a better way to do this later.

### 3.3 Potential Problems

#### 1. Non-linearity of response-predictor relationships

diagnosis:  
 plot residuals vs. fitted values → or each predictor  
 see pattern.

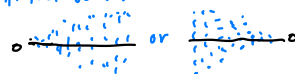
solution  
 - add polynomial term  
 - transform predictor

#### 2. Correlation of error terms

diagnosis:  
 understanding how data is collected.  
 time series? spatial data?

solution  
 ✗ use models formulated for correlated errors (not this class)  
 - include a predictor to capture dependence.

#### 3. Non-constant variance of error terms

diagnosis  
 plot residuals vs. fitted values  
 see funnel pattern 

solution  
 transform Y. Try  $\log Y$  or  $\sqrt{Y}$

#### 4. Outliers

diagnosis  
 plot data

solution  
 Is your data wrong? i.e. error in data collection?  
 fix it.

otherwise - maybe you are missing a predictor?

## 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  $f(X)$ .

easy to fit  
easy to interpret  
can do hypothesis testing.

make strong assumptions, what if they are wrong?  
- parametric model will perform poorly.

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

Given a value for *K* (← # of neighbors) 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  $\mathcal{N}_0$ , (→ neighborhood)

$$\hat{f}(x_0) = \frac{1}{K} \sum_{x_i \in \mathcal{N}_0} y_i$$

value to be predicted. (pointing to  $\hat{f}(x_0)$ )  
training data (pointing to  $y_i$ )

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 <- data.frame(x = x, y = y) # data frame of training data

for (k in seq(2, 10, by = 2)) {  
    ← K = 2, 4, 6, 8, 10

    nearest\_neighbor(mode = "regression", neighbors = k) |>

    fit(y ~ 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 ~ x, df) |>

augment(new\_data = df) |>

ggplot() +

geom\_point(aes(x, y)) +

geom\_line(aes(x, .pred), colour = "red") +

generate  
fake data

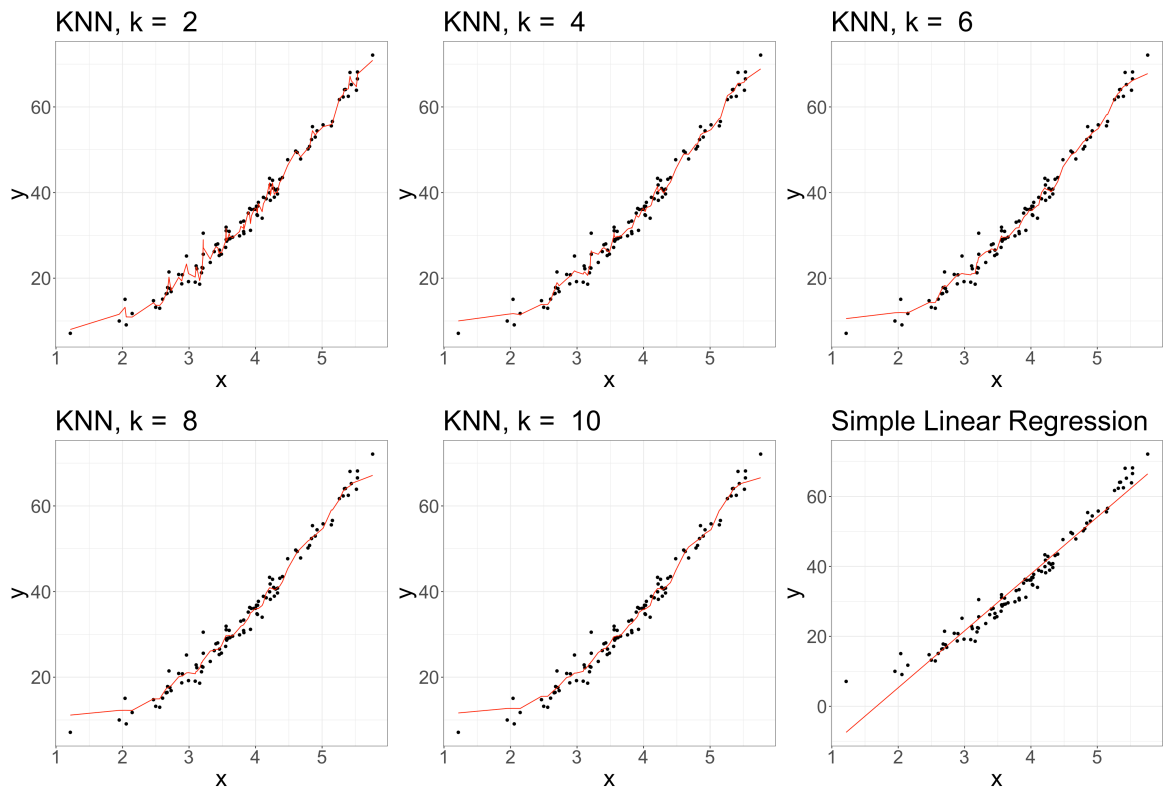
model  
specification  
fit model

formula  
just like  
before.

add predicted values + residuals. to the data frame "new\_data"

compare  
to  
linear model

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



as  $k \uparrow$ , KNN fitted line gets smoother

↑  
missing quadratic relationship.