Machine Learning: Regression in R

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Why a part on simple regression

- OLS can be seen as a simple machine learning technique
- Some other machine learning concepts are based on regression (e.g. regularization).
- We would like to remind you how simple regression works in R.
- We also want to show the constraints
- In a next step we will learn, how to coop with these constraints

Variables of the `mtcars` dataset

Help for the `mtcars` dataset:

```
?mtcars
```

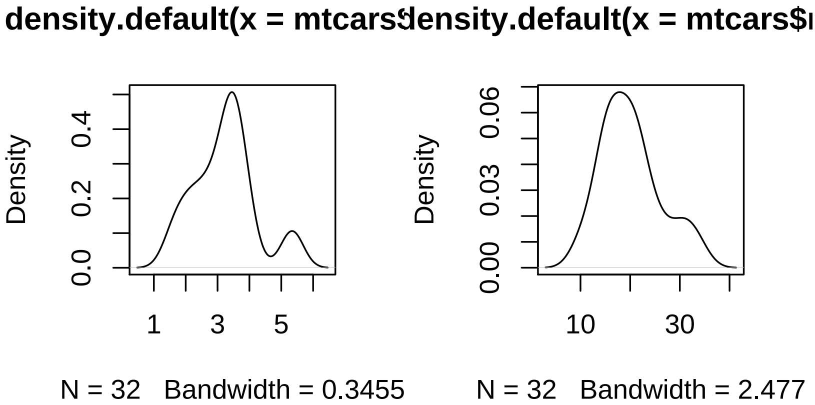
- mpg - Miles/(US) gallon
- cyl - Number of cylinders
- disp - Displacement (cu.in.)
- hp - Gross horsepower
- drat - Rear axle ratio
- wt - Weight (1000 lbs)
- qsec - 1/4 mile time
- vs - Engine (0 = V-shaped, 1 = straight)
- am - Transmission (0 = automatic, 1 = manual)
- gear - Number of forward gears
- carb - Number of carburetors

Dataset mtcars

	mpg	cyl	disp	hp	drat	wt	qsec	vs	ar
Mazda RX4	21.0	6	160.0	110	3.90	2.620	16.46	0	
Mazda RX4 Wag	21.0	6	160.0	110	3.90	2.875	17.02	0	
Datsun 710	22.8	4	108.0	93	3.85	2.320	18.61	1	
Hornet 4 Drive	21.4	6	258.0	110	3.08	3.215	19.44	1	
Hornet Sportabout	18.7	8	360.0	175	3.15	3.440	17.02	0	
Valiant	18.1	6	225.0	105	2.76	3.460	20.22	1	
Duster 360	14.3	8	360.0	245	3.21	3.570	15.84	0	
Merc 240D	24.4	4	146.7	62	3.69	3.190	20.00	1	
Merc 230	22.8	4	140.8	95	3.92	3.150	22.90	1	
Merc 280	19.2	6	167.6	123	3.92	3.440	18.30	1	
Merc 280C	17.8	6	167.6	123	3.92	3.440	18.90	1	
Merc 450SE	16.4	8	275.8	180	3.07	4.070	17.40	0	
Merc 450SL	17.3	8	275.8	180	3.07	3.730	17.60	0	
Merc 450SLC	15.2	8	275.8	180	3.07	3.780	18.00	0	
Cadillac Fleetwood	10.4	8	472.0	205	2.93	5.250	17.98	0	
Lincoln Continental	10.4	8	460.0	215	3.00	5.424	17.82	0	

Distributions of two variables of mtcars

```r
par(mfrow=c(1,2))
plot(density(mtcars$wt)); plot(density(mtcars$mpg))
```



A simple regression model

Dependent variable - miles per gallon (mpg)

Independent variable - weight (wt)

```
m1 <- lm(mpg ~ wt,data=mtcars)
m1
##
## Call:
## lm(formula = mpg ~ wt, data = mtcars)
##
## Coefficients:
## (Intercept)           wt
##      37.285       -5.344
```

Get the model summary

```
summary(m1)
```

```
##
## Call:
## lm(formula = mpg ~ wt, data = mtcars)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -4.5432 -2.3647 -0.1252  1.4096  6.8727
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  37.2851     1.8776  19.858  < 2e-16 ***
## wt           -5.3445     0.5591  -9.559 1.29e-10 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' '
##
## Residual standard error: 3.046 on 30 degrees of freedom
```

The model formula

Model without intercept

```r
m2 <- lm(mpg ~ - 1 + wt,data=mtcars)
summary(m2)$coefficients
##    Estimate Std. Error  t value     Pr(>|t|)
## wt 5.291624  0.5931801 8.920771 4.55314e-10
```

Adding further variables

```r
m3 <- lm(mpg ~ wt + cyl,data=mtcars)
summary(m3)$coefficients
##              Estimate Std. Error   t value     Pr(>|t|)
## (Intercept) 39.686261  1.7149840 23.140893 3.043182e-20
## wt          -3.190972  0.7569065 -4.215808 2.220200e-04
## cyl         -1.507795  0.4146883 -3.635972 1.064282e-03
```

The command as.formula

```
?as.formula
```

```
class(fo <- mpg ~ wt + cyl)
```

```
## [1] "formula"
```

```
# The formula object can be used in the regression:
m3 <- lm(fo,data=mtcars)
```

Further possibilities to specify the formula

Take all available predictors

```
m3_a<-lm(mpg~.,data=mtcars)
```

Interaction effect

```
# effect of cyl and interaction effect:
m3a<-lm(mpg~wt*cyl,data=mtcars)

# only interaction effect:
m3b<-lm(mpg~wt:cyl,data=mtcars)
```

Take the logarithm

```
m3d<-lm(mpg~log(wt),data=mtcars)
```

The command setdiff

- We can use the command to create a dataset with only the features, without the dependent variable

```
names(mtcars)
```

```
##  [1] "mpg"  "cyl"  "disp" "hp"   "drat" "wt"   "qsec" "vs"
## [11] "carb"
```

```
features <- setdiff(names(mtcars), "mpg")
features
```

```
##  [1] "cyl"  "disp" "hp"   "drat" "wt"   "qsec" "vs"   "am"
```

```
featdat <- mtcars[,features]
```

The command model.matrix

- With `model.matrix` the qualitative variables are automatically dummy encoded

```
?model.matrix
```

```
model.matrix(m3d)
```

```
##                     (Intercept)   log(wt)
## Mazda RX4                     1 0.9631743
## Mazda RX4 Wag                 1 1.0560527
## Datsun 710                    1 0.8415672
## Hornet 4 Drive                1 1.1678274
## Hornet Sportabout             1 1.2354715
## Valiant                       1 1.2412686
## Duster 360                    1 1.2725656
## Merc 240D                     1 1.1600209
## Merc 230                      1 1.1474025
## Merc 280                      1 1.2354715
## Merc 280C                     1 1.2354715
```

Model matrix (II)

- We can also create a model matrix directly from the formula and data arguments
- See `Matrix::sparse.model.matrix` for increased efficiency on large dimension data.

```
ff <- mpg ~ log(wt):cyl
m <- model.frame(ff, mtcars)
```

```
(mat <- model.matrix(ff, m))
```

```
##                     (Intercept) log(wt):cyl
## Mazda RX4                     1    5.779046
## Mazda RX4 Wag                 1    6.336316
## Datsun 710                    1    3.366269
## Hornet 4 Drive                1    7.006964
## Hornet Sportabout             1    9.883772
## Valiant                       1    7.447612
## Duster 360                    1   10.180525
## Merc 240D                     1    4.640084
```

A model with interaction effect

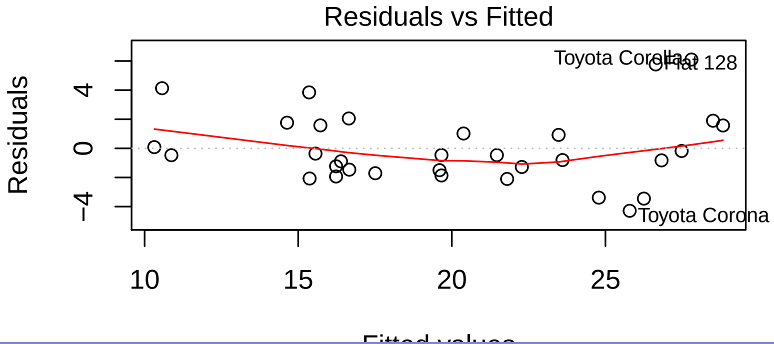
```r
# disp  -  Displacement (cu.in.)
m3d<-lm(mpg~wt*disp,data=mtcars)
m3dsum <- summary(m3d)
m3dsum$coefficients
```

```
##                Estimate  Std. Error   t value     Pr(>|t|)
## (Intercept) 44.08199770 3.123062627 14.114990 2.955567e-14
## wt          -6.49567966 1.313382622 -4.945763 3.216705e-05
## disp        -0.05635816 0.013238696 -4.257078 2.101721e-04
## wt:disp      0.01170542 0.003255102  3.596022 1.226988e-03
```

Residual plot - model assumptions violated?

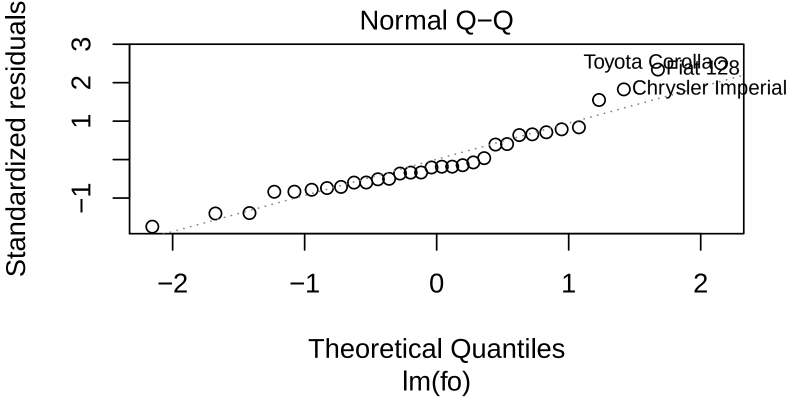
- We have model assumptions violated if points deviate with a pattern from the line

```
plot(m3,1)
```



Residual plot

```r
plot(m3,2)
```



Another example for object orientation

- m3 is now a special regression object
- Various functions can be applied to this object

```
predict(m3) # Prediction
resid(m3) # Residuals
```

```
##          Mazda RX4      Mazda RX4 Wag         Datsun 710    Horn
##           22.27914           21.46545           26.25203
## Hornet Sportabout            Valiant
##           16.64696           19.59873
```

```
##          Mazda RX4      Mazda RX4 Wag         Datsun 710    Horn
##         -1.2791447         -0.4654468         -3.4520262
## Hornet Sportabout            Valiant
##          2.0530424         -1.4987281
```

Make model prediction

```r
pre <- predict(m1)
head(mtcars$mpg)
```

```
## [1] 21.0 21.0 22.8 21.4 18.7 18.1
```

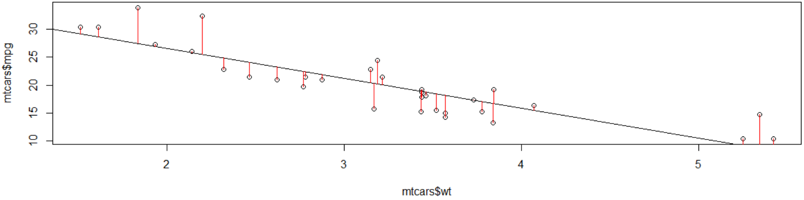
```r
head(pre)
```

```
##         Mazda RX4     Mazda RX4 Wag        Datsun 710    Horn
##          23.28261          21.91977          24.88595
## Hornet Sportabout           Valiant
##          18.90014          18.79325
```

Regression diagnostic with base-R

Visualizing residuals

```
plot(mtcars$wt,mtcars$mpg)
abline(m1)
segments(mtcars$wt, mtcars$mpg, mtcars$wt, pre, col="red")
```



The mean squared error (mse)

- The **MSE** measures the average of the squares of the errors
- **The lower the better**

```
(mse5 <- mean((mtcars$mpg -  pre)^2)) # model 5
```

```
## [1] 8.697561
```

```
(mse3 <- mean((mtcars$mpg -  predict(m3))^2))
```

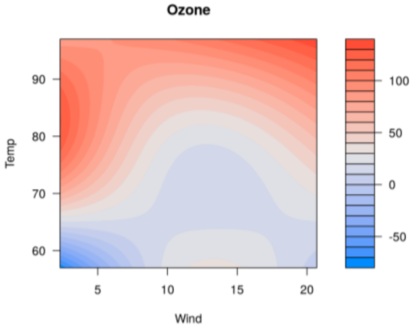
```
## [1] 5.974124
```

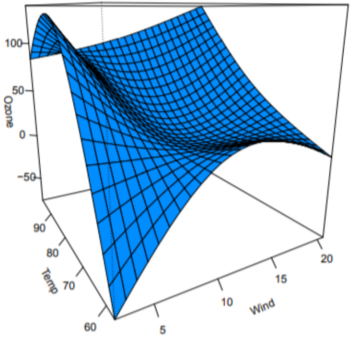
Package Metrics to compute mse

```
library(Metrics)
mse(mtcars$mpg,predict(m3))
## [1] 5.974124
```

The visreg-package

```
install.packages("visreg")
library(visreg)
```

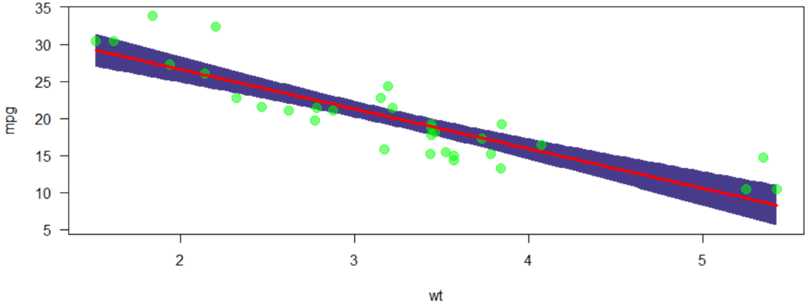




The visreg-package

- The default-argument for `type` is `conditional`.
- Scatterplot of `mpg` and `wt` plus regression line and confidence bands

```
visreg(m1, "wt", type = "conditional")
```



Regression with factors

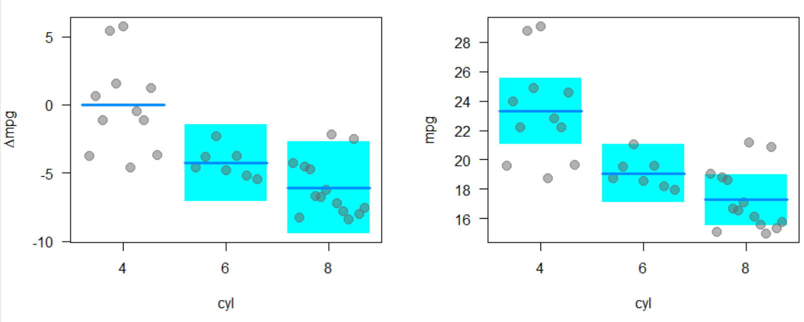
- The effects of factors can also be visualized with visreg:

```
mtcars$cyl <- as.factor(mtcars$cyl)
m4 <- lm(mpg ~ cyl + wt, data = mtcars)
# summary(m4)
```

```
##              Estimate Std. Error   t value     Pr(>|t|)
## (Intercept) 33.990794  1.8877934 18.005569 6.257246e-17
## cyl6        -4.255582  1.3860728 -3.070244 4.717834e-03
## cyl8        -6.070860  1.6522878 -3.674214 9.991893e-04
## wt          -3.205613  0.7538957 -4.252065 2.130435e-04
```

Effects of factors

```
par(mfrow=c(1,2))
visreg(m4, "cyl", type = "contrast")
visreg(m4, "cyl", type = "conditional")
```



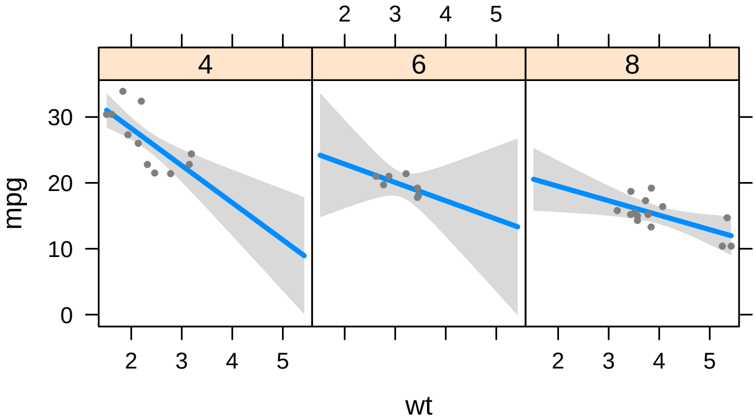
The package visreg - Interactions

```
m5 <- lm(mpg ~ cyl*wt, data = mtcars)
# summary(m5)
```

```
##              Estimate Std. Error   t value     Pr(>|t|)
## (Intercept)  39.571196   3.193940 12.3894599 2.058359e-12
## cyl6        -11.162351   9.355346 -1.1931522 2.435843e-01
## cyl8        -15.703167   4.839464 -3.2448150 3.223216e-03
## wt           -5.647025   1.359498 -4.1537586 3.127578e-04
## cyl6:wt       2.866919   3.117330  0.9196716 3.661987e-01
## cyl8:wt       3.454587   1.627261  2.1229458 4.344037e-02
```

Control of the graphic output with `layout`.

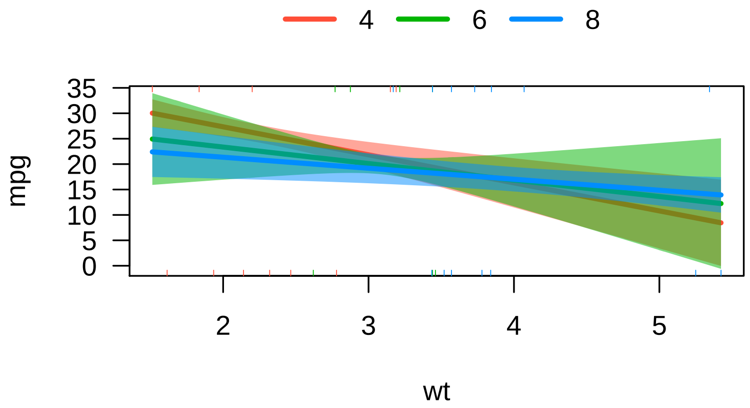
```
visreg(m5, "wt", by = "cyl",layout=c(3,1))
```



The package visreg - Interactions overlay

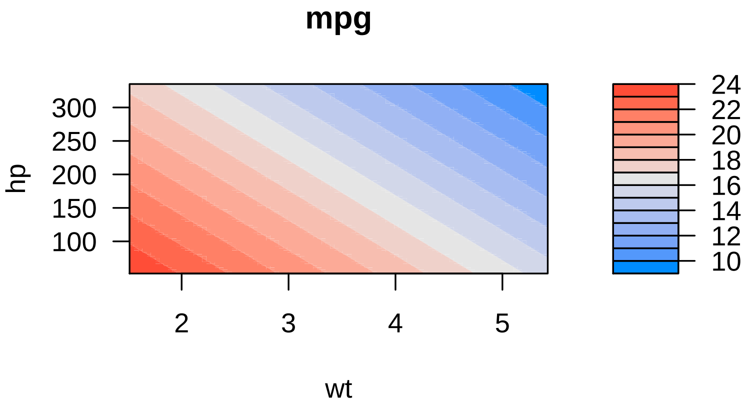
```
m6 <- lm(mpg ~ hp + wt * cyl, data = mtcars)

visreg(m6, "wt", by="cyl", overlay=TRUE, partial=FALSE)
```



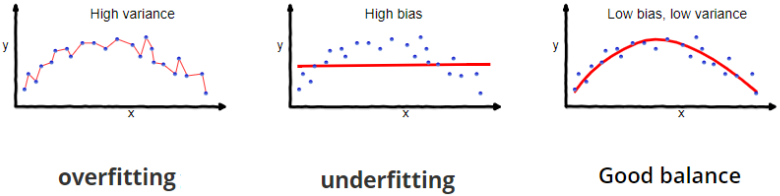
The package visreg - visreg2d

```
visreg2d(m6, "wt", "hp", plot.type = "image")
```

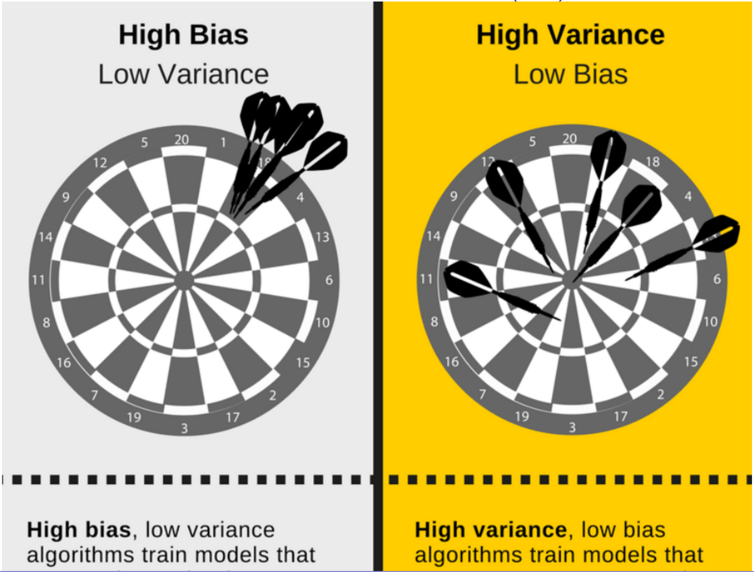


The bias-variance tradeoff (I)

- The bias–variance tradeoff is the property of a set of predictive models whereby models with a lower bias in parameter estimation have a higher variance of the parameter estimates across samples, and vice versa.



The bias-variance tradeoff (II)



Exercise: regression Ames housing data

1) Install the package `AmesHousing` and create a **processed version** of the Ames housing data with (at least) the variables `Sale_Price`, `Gr_Liv_Area` and `TotRms_AbvGrd`
2) Create a regression model with `Sale_Price` as dependent and `Gr_Liv_Area` and `TotRms_AbvGrd` as independent variables. Then create seperated models for the two independent variables. Compare the results. What do you think?

The Ames Iowa Housing Data

```
ames_data <- AmesHousing::make_ames()
```

Some Variables

- `Gr_Liv_Area`: Above grade (ground) living area square feet
- `TotRms_AbvGrd`: Total rooms above grade (does not include bathrooms
- `MS_SubClass`: Identifies the type of dwelling involved in the sale.
- `MS_Zoning`: Identifies the general zoning classification of the sale.
- `Lot_Frontage`: Linear feet of street connected to property
- `Lot_Area`: Lot size in square feet
- `Street`: Type of road access to property
- `Alley`: Type of alley access to property
- `Lot_Shape`: General shape of property
- `Land_Contour`: Flatness of the propert

Multicollinearity

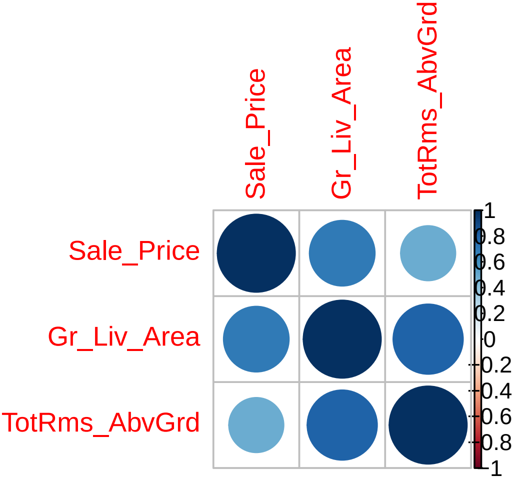
- As p increases we are more likely to capture multiple features that have some multicollinearity.
- When multicollinearity exists, we often see high variability in our coefficient terms.
- E.g. we have a correlation of 0.801 between `Gr_Liv_Area` and `TotRms_AbvGrd`
- Both variables are strongly correlated to the response variable (`Sale_Price`).

```
ames_data <- AmesHousing::make_ames()
cor(ames_data[,c("Sale_Price","Gr_Liv_Area","TotRms_AbvGrd")])
```

```
##               Sale_Price Gr_Liv_Area TotRms_AbvGrd
## Sale_Price     1.0000000   0.7067799     0.4954744
## Gr_Liv_Area    0.7067799   1.0000000     0.8077721
## TotRms_AbvGrd  0.4954744   0.8077721     1.0000000
```

A correlation plot

```
library(corrplot)
corrplot(cor(ames_data[,c("Sale_Price","Gr_Liv_Area","TotRms_Abv
```



Multicollinearity

```
lm(Sale_Price ~ Gr_Liv_Area + TotRms_AbvGrd, data = ames_data)
```

```
##
## Call:
## lm(formula = Sale_Price ~ Gr_Liv_Area + TotRms_AbvGrd, data =
##
## Coefficients:
##   (Intercept)    Gr_Liv_Area  TotRms_AbvGrd
##       42767.6          139.4       -11025.9
```

- When we fit a model with both these variables we get a positive coefficient for `Gr_Liv_Area` but a negative coefficient for `TotRms_AbvGrd`, suggesting one has a positive impact to Sale_Price and the other a negative impact.

Seperated models

- If we refit the model with each variable independently, they both show a positive impact.
- The Gr_Liv_Area effect is now smaller and the TotRms_AbvGrd is positive with a much larger magnitude.

```
lm(Sale_Price ~ Gr_Liv_Area, data = ames_data)$coefficients
```

```
## (Intercept) Gr_Liv_Area
##   13289.634     111.694
```

```
lm(Sale_Price ~ TotRms_AbvGrd, data = ames_data)$coefficients
```

```
##   (Intercept) TotRms_AbvGrd
##      18665.40      25163.83
```

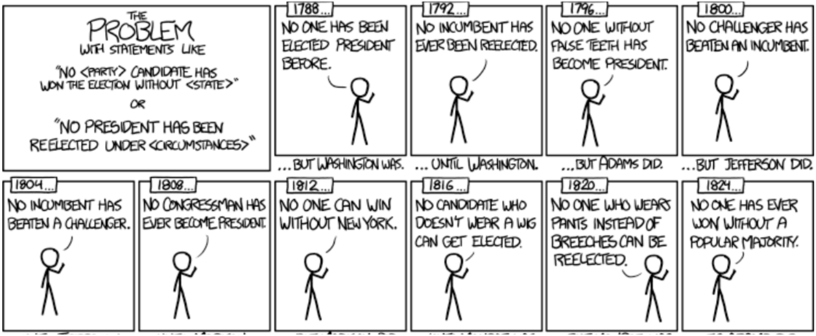
- This is a common result when collinearity exists.
- Coefficients for correlated features become over-inflated and can fluctuate significantly.

Consequences

- One consequence of these large fluctuations in the coefficient terms is **overfitting**, which means we have high variance in the bias-variance tradeoff space.
- We can use tools such as **variance inflaction factors** (Myers, 1994) to identify and remove those strongly correlated variables, but it is not always clear which variable(s) to remove.
- Nor do we always wish to remove variables as this may be removing signal in our data.

The problem - Overfitting

- Our model doesn't generalize well from our training data to unseen data.



What can be done against overvitting

- **Cross Validation**
- Train with more data
- Remove features
- Regularization - e.g. ridge and lasso regression
- Ensembling - e.g. bagging and boosting

Cross validation

- Cross-validation is a powerful preventative measure against overfitting.
- Use your initial training data to generate multiple mini train-test splits. Use these splits to tune your model.

Necessary packages

```
library(tidyverse)
library(caret)
```

Cross Validation in R

Split data into training and testing dataset

```
training.samples <- ames_data$Sale_Price %>%
createDataPartition(p = 0.8, list = FALSE)
train.data  <- ames_data[training.samples, ]
test.data <- ames_data[-training.samples, ]
```

Build the model and make predictions

```
model <- lm(Sale_Price ~ Gr_Liv_Area + TotRms_AbvGrd,
            data = train.data)
# Make predictions and compute the R2, RMSE and MAE
(predictions <- model %>% predict(test.data))
##         1         2         3         4         5         6
## 165512.95 173881.44 365431.71 212681.67 140216.52 124165.47 1
##         9        10        11        12        13        14
## 167242.64 308218.57 198110.03 167624.54 180907.72 225165.81 1
##        17        18        19        20        21        22
## 112558.22 269698.29 165155.15 170093.93 205709.16 222201.43 1
##        25        26        27        28        29        30
```

Model with cross validation

- Loocv: **leave one out cross validation**

```
train.control <- caret::trainControl(method = "LOOCV")
```

```
# Train the model
model2 <- train(Sale_Price ~ Gr_Liv_Area + TotRms_AbvGrd,
                data = train.data, method = "lm",
                trControl = train.control)
model2 %>% predict(test.data)
```

Links - linear regression

- Regression - **r-bloggers**
- The complete book of **Faraway**- very intuitive
- Good introduction on **Quick-R**
- **Multiple regression**
- **15 Types of Regression you should know**
- `ggeffects` - **Create Tidy Data Frames of Marginal Effects for 'ggplot' from Model Outputs**
- **Machine learning iteration**

Nice table output with stargazer

```r
library(stargazer)
stargazer(m3, type="html")
```

Example HTML output:

	Dependent variable:
	mpg
wt	-3.125***
	(0.911)
cyl	-1.510***
	(0.422)
am	0.176
	(1.304)
Constant	39.418***
	(2.641)
Observations	32
R^2	0.830

Shiny App - Diagnostics for linear regression

- Shiny App - **Simple Linear Regression**
- Shiny App - **Multicollinearity in multiple regression**