Machine Learning and Data Analytics
ME 5013- Fall 2019

Lecture 04

- Multiple Linear Regression

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Disclosure: Slides are adopted from Drs. Hastie and Tibshirani on "Statistical Learning" at Stanford university

- Here our model is

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \epsilon,$$

- We interpret β_j as the *average* effect on Y of a one unit increase in X_j, *holding all other predictors fixed*. In the advertising example, the model becomes

$$\mathit{sales} = \beta_0 + \beta_1 \times \mathit{TV} + \beta_2 \times \mathit{radio} + \beta_3 \times \mathit{newspaper} + \epsilon.$$

Interpreting regression coefficients

- The ideal scenario is when the predictors are uncorrelated — a *balanced design*:
  - Each coefficient can be estimated and tested separately.
  - Interpretations such as *"a unit change in X_j is associated with a β_j change in Y, while all the other variables stay fixed"*, are possible.
- Correlations amongst predictors cause problems:
  - The variance of all coefficients tends to increase, sometimes dramatically
  - Interpretations become hazardous — when X_j changes, everything else changes.
- *Claims of causality* should be avoided for observational data.

"Data Analysis and Regression" Mosteller and Tukey 1977

- A regression coefficient β_j estimates the expected change in Y per unit change in X_j, *with all other predictors held fixed*. But predictors usually change together!

- Example: Y total amount of change in your pocket;

  X_1 = # of coins; X_2 = # of pennies, nickels and dimes. By itself, regression coefficient of Y on X_2 will be > 0. But how about with X_1 in model?

- Y = number of tackles by a football player in a season; W and H are his weight and height. Fitted regression model is $\hat{Y} = b_0 + 0.5W - 0.1H$. How do we interpret $\hat{\beta}_2 < 0$?

Two quotes by famous Statisticians

"Essentially, all models are wrong, but some are useful"

George Box

"The only way to find out what will happen when a complex system is disturbed is to disturb the system, not merely to observe it passively"

Fred Mosteller and John Tukey, paraphrasing George Box

Estimation and Prediction for Multiple Regression

- Given estimates $\hat{\beta}_0, \hat{\beta}_1, \ldots \hat{\beta}_p$, we can make predictions using the formula

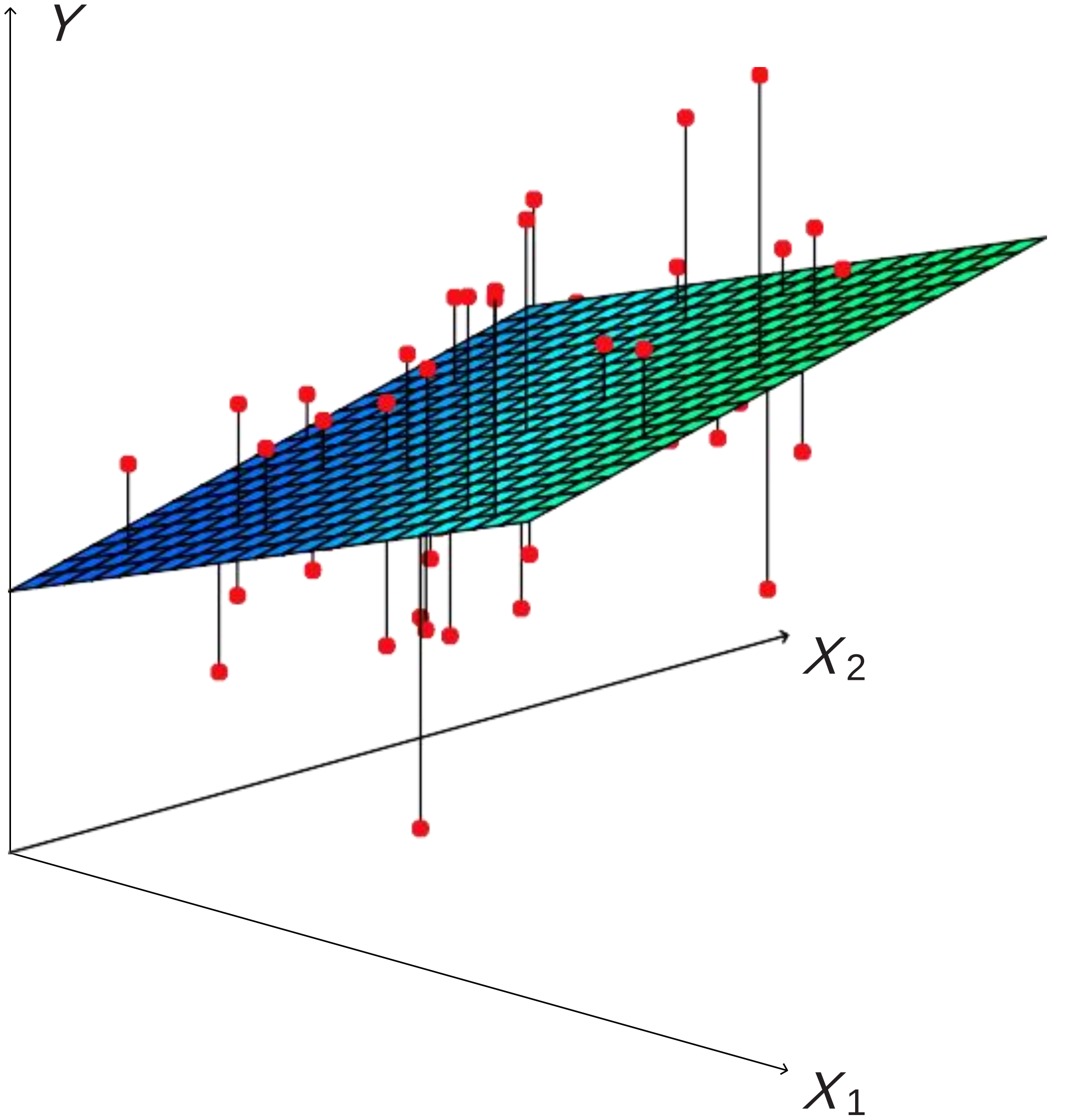
$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 + \cdots + \hat{\beta}_p x_p$$

- We estimate $\beta_0, \beta_1, \ldots, \beta_p$ as the values that minimize the sum of squared residuals

$$\begin{aligned} \mathrm{RSS} &= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} - \hat{\beta}_2 x_{i2} - \cdots - \hat{\beta}_p x_{ip})^2. \end{aligned}$$

This is done using standard statistical software. The values $\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p$ that minimize RSS are the multiple least squares regression coefficient estimates.

Estimation and Prediction for Multiple Regression



Results for advertising data

	Coefficient	Std. Error	t-statistic	p-value
Intercept	2.939	0.3119	9.42	< 0.0001
TV	0.046	0.0014	32.81	< 0.0001
radio	0.189	0.0086	21.89	< 0.0001
newspaper	-0.001	0.0059	-0.18	0.8599

Correlation

	TV	radio	newspaper	sales
TV	1.0000	0.0548	0.0567	0.7822
radio		1.0000	0.3541	0.5762
newspaper			1.0000	0.2283
sales				1.0000

Some important questions

1. Is at least one of the predictors $X_1, X_2, \ldots, X_p$ useful in predicting the response?
2. Do all the predictors help to explain Y , or is only a subset of the predictors useful?
3. How well does the model fit the data?
4. Given a set of predictor values, what response value should we predict, and how accurate is our prediction?

Is at least one predictor useful?

$$F = \frac{(\mathrm{TSS} - \mathrm{RSS})/p}{\mathrm{RSS}/(n-p-1)} \sim F_{p,n-p-1}$$

Quantity	Value
Residual Standard Error	1.69
R^2	0.897
F-statistic	570

Deciding on important variables

- The most direct approach is called all subsets or best subsets regression: we compute the least squares fit for all possible subsets and then choose between them based on some criterion that balances training error with model size.
- However we often can't examine all possible models, since they are 2^p of them; for example when p = 40 there are over a billion models!
- Instead we need an automated approach that searches through a subset of them. We discuss two commonly use approaches next.

Forward selection

- Begin with the *null model* — a model that contains an intercept but no predictors.
- Fit *p* simple linear regressions and add to the null model the variable that results in the lowest RSS.
- Add to that model the variable that results in the lowest RSS amongst all two-variable models.
- Continue until some stopping rule is satisfied, for example when all remaining variables have a p-value above some threshold.

Backward selection

- Start with all variables in the model.
- Remove the variable with the largest p-value — that is, the variable that is the least statistically significant.
- The new ($p-1$)-variable model is fit, and the variable with the largest p-value is removed.
- Continue until a stopping rule is reached. For instance, we may stop when all remaining variables have a significant p-value defined by some significance threshold.

Model selection — continued

- Later we discuss more systematic criteria for choosing an "optimal" member in the path of models produced by forward or backward stepwise selection.

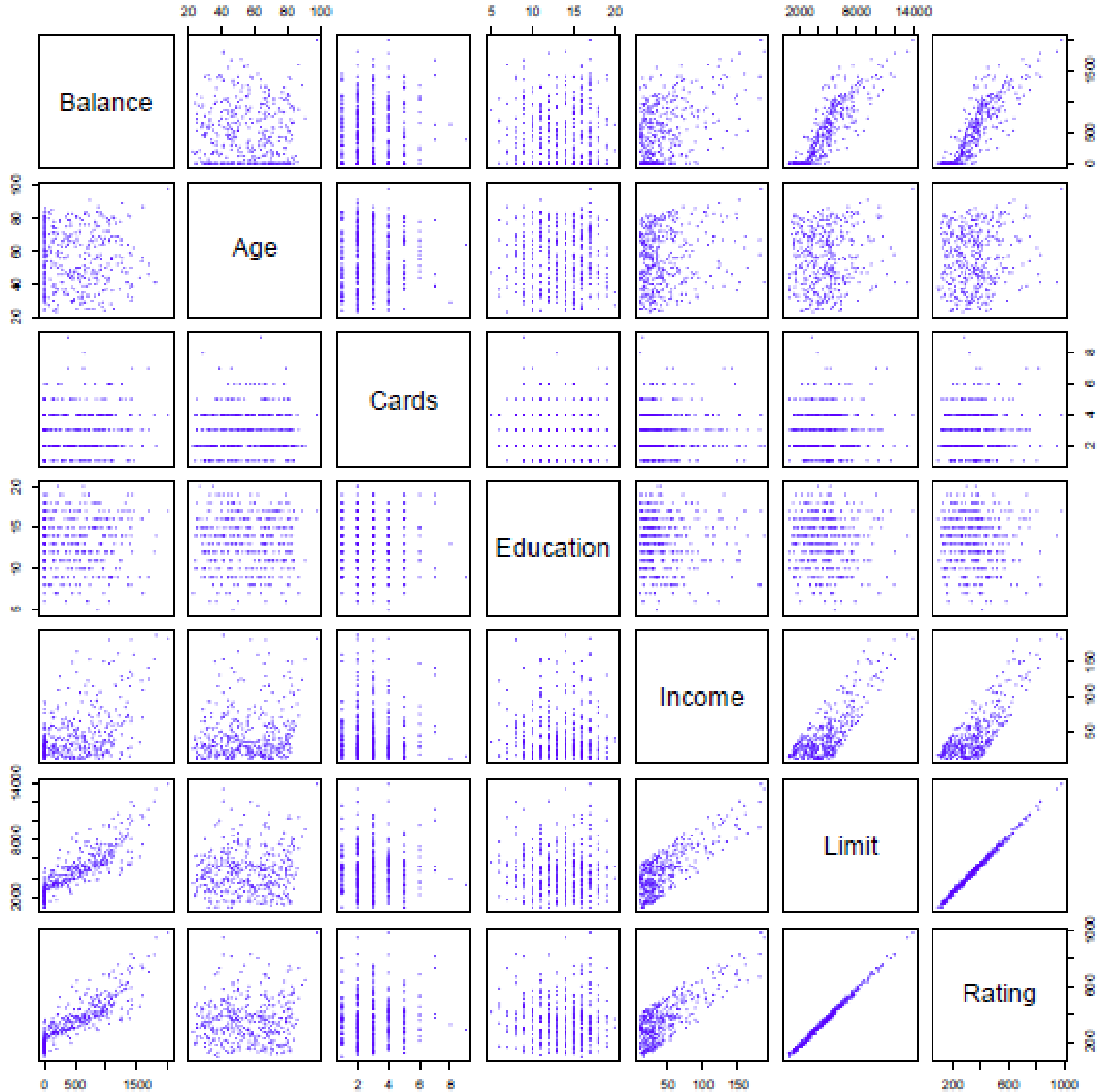
- These include *Mallow's C_p*, *Akaike information criterion (AIC)*, *Bayesian information criterion (BIC)*, *adjusted R^2* and *Cross-validation (CV)*.

Qualitative Predictors

- Some predictors are not *quantitative* but are *qualitative*, taking a discrete set of values.
- These are also called *categorical* predictors or *factor variables*.
- See for example the scatterplot matrix of the credit card data in the next slide.

In addition to the 7 quantitative variables shown, there are four qualitative variables: gender, student (student status), status (marital status), and ethnicity (Caucasian, African American (AA) or Asian).

Credit Card Data



Qualitative Predictors — continued

Example: investigate differences in credit card balance between males and females, ignoring the other variables. We create a new variable

$$x_i = \begin{cases} 1 & \text{if } i\text{th person is female} \\ 0 & \text{if } i\text{th person is male.} \end{cases}$$

Resulting model:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i = \begin{cases} \beta_0 + \beta_1 + \epsilon_i & \text{if } i\text{th person is female} \\ \beta_0 + \epsilon_i & \text{if } i\text{th person is male.} \end{cases}$$

Intrepretatio?

Credit card data — continued

Results for gender model:

	Coefficient	Std. Error	t-statistic	p-value
Intercept	509.80	33.13	15.389	< 0.0001
gender[Female]	19.73	46.05	0.429	0.6690

Qualitative predictors with more than two levels

- With more than two levels, we create additional dummy variables. For example, for the ethnicity variable we create two dummy variables. The first could be

$$x_{i1} = \begin{cases} 1 & \text{if } i\text{th person is Asian} \\ 0 & \text{if } i\text{th person is not Asian,} \end{cases}$$

and the second could be

$$x_{i2} = \begin{cases} 1 & \text{if } i\text{th person is Caucasian} \\ 0 & \text{if } i\text{th person is not Caucasian.} \end{cases}$$

Qualitative predictors with more than two levels — continued.

- Then both of these variables can be used in the regression equation, in order to obtain the model

$$y_i = \beta_0+\beta_1 x_{i1}+\beta_2 x_{i2}+\epsilon_i = \begin{cases} \beta_0+\beta_1+\epsilon_i & \text{if } i\text{th person is Asian} \\ \beta_0+\beta_2+\epsilon_i & \text{if } i\text{th person is Caucasian} \\ \beta_0+\epsilon_i & \text{if } i\text{th person is AA.} \end{cases}$$

- There will always be one fewer dummy variable than the number of levels. The level with no dummy variable — African American in this example — is known as the *baseline*.

Results for ethnicity

	Coefficient	Std. Error	t-statistic	p-value
Intercept	531.00	46.32	11.464	< 0.0001
ethnicity[Asian]	-18.69	65.02	-0.287	0.7740
ethnicity[Caucasian]	-12.50	56.68	-0.221	0.8260

Removing the additive assumption: *interactions* and *nonlinearity*

Interactions:

- In our previous analysis of the Advertising data, we assumed that the effect on sales of increasing one advertising medium is independent of the amount spent on the other media.
- For example, the linear model

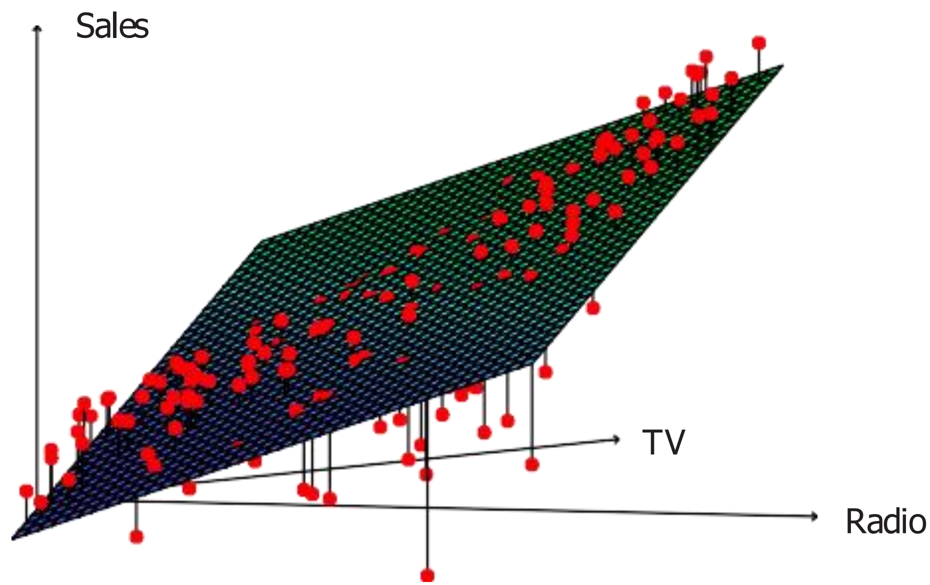
$$\widehat{sales} = \beta_0 + \beta_1 \times TV + \beta_2 \times radio + \beta_3 \times newspaper$$

  states that the average effect on sales of a one-unit increase in TV is always β_1, regardless of the amount spent on radio.

Interactions — continued

- But suppose that spending money on radio advertising actually increases the effectiveness of TV advertising, so that the slope term for TV should increase as radio increases.
- In this situation, given a fixed budget of $100, 000, spending half on radio and half on TV may increase sales more than allocating the entire amount to either TV or to radio.
- In marketing, this is known as a *synergy* effect, and in statistics it is referred to as an *interaction* effect.

Interaction in the Advertising data?



When levels of either TV or radio are low, then the true sales are lower than predicted by the linear model.
But when advertising is split between the two media, then the model tends to underestimate sales.

Modelling interactions — Advertising data

Model takes the form

$$\begin{aligned} sales &= \beta_0 + \beta_1 \times TV + \beta_2 \times radio + \beta_3 \times (radio \times TV) + \epsilon \\ &= \beta_0 + (\beta_1 + \beta_3 \times radio) \times TV + \beta_2 \times radio + \epsilon \end{aligned}$$

Results:

	Coefficient	Std. Error	t-statistic	p-value
Intercept	6.7502	0.248	27.23	< 0.0001
TV	0.0191	0.002	12.70	< 0.0001
radio	0.0289	0.009	3.24	0.0014
TV×radio	0.0011	0.000	20.73	< 0.0001

Interpretation

- The results in this table suggests that interactions are important.
- The p-value for the interaction term TV×radio is extremely low, indicating that there is strong evidence for $H_A : \beta_3 \neq 0$.
- The R^2 for the interaction model is 96.8%, compared to only 89.7% for the model that predicts sales using TV and radio without an interaction term.

Interpretation — continued

- This means that (96.8 − 89.7)/(100 − 89.7) = 69% of the variability in sales that remains after fitting the additive model has been explained by the interaction term.

- The coefficient estimates in the table suggest that an increase in TV advertising of $1, 000 is associated with increased sales of

  $(\hat{\beta}_1 + \hat{\beta}_3 \times radio) \times 1000 = 19 + 1.1 \times radio$ units.

- An increase in radio advertising of $1, 000 will be associated with an increase in sales of

  $(\hat{\beta}_2 + \hat{\beta}_3 \times TV) \times 1000 = 29 + 1.1 \times TV$ units.

Hierarchy

- Sometimes it is the case that an interaction term has a very small p-value, but the associated main effects (in this case, TV and radio) do not.
- The *hierarchy principle*:

  If we include an interaction in a model, we should also include the main effects, even if the p-values associated with their coefficients are not significant.
- The rationale for this principle is that interactions are hard to interpret in a model without main effects — their meaning is changed.
- Specifically, the interaction terms also contain main effects, if the model has no main effect terms.

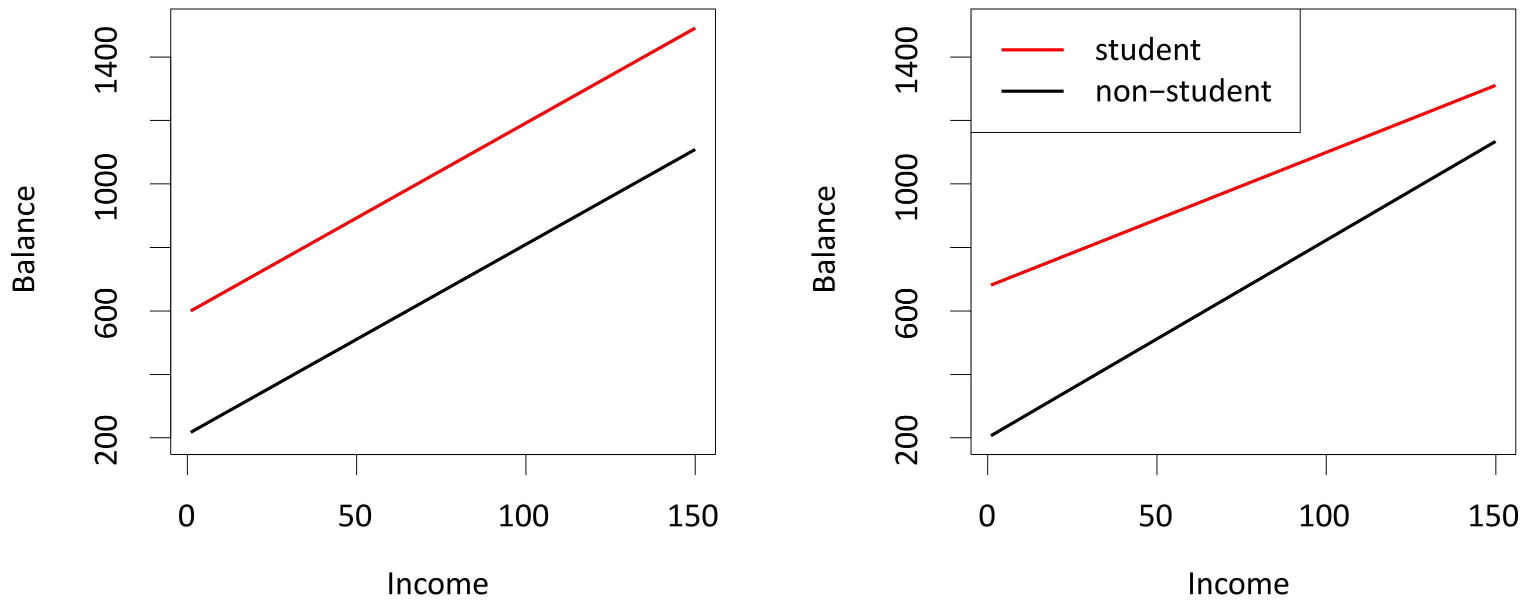
Interactions between qualitative and quantitative variables

Consider the Credit data set, and suppose that we wish to predict balance using income (quantitative) and student (qualitative).

Without an interaction term, the model takes the form

$$
\begin{aligned}
\texttt{balance}_i &\approx \beta_0 + \beta_1 \times \texttt{income}_i + \begin{cases} \beta_2 & \text{if } i\text{th person is a student} \\ 0 & \text{if } i\text{th person is not a student} \end{cases} \\
&= \beta_1 \times \texttt{income}_i + \begin{cases} \beta_0 + \beta_2 & \text{if } i\text{th person is a student} \\ \beta_0 & \text{if } i\text{th person is not a student.} \end{cases}
\end{aligned}
$$

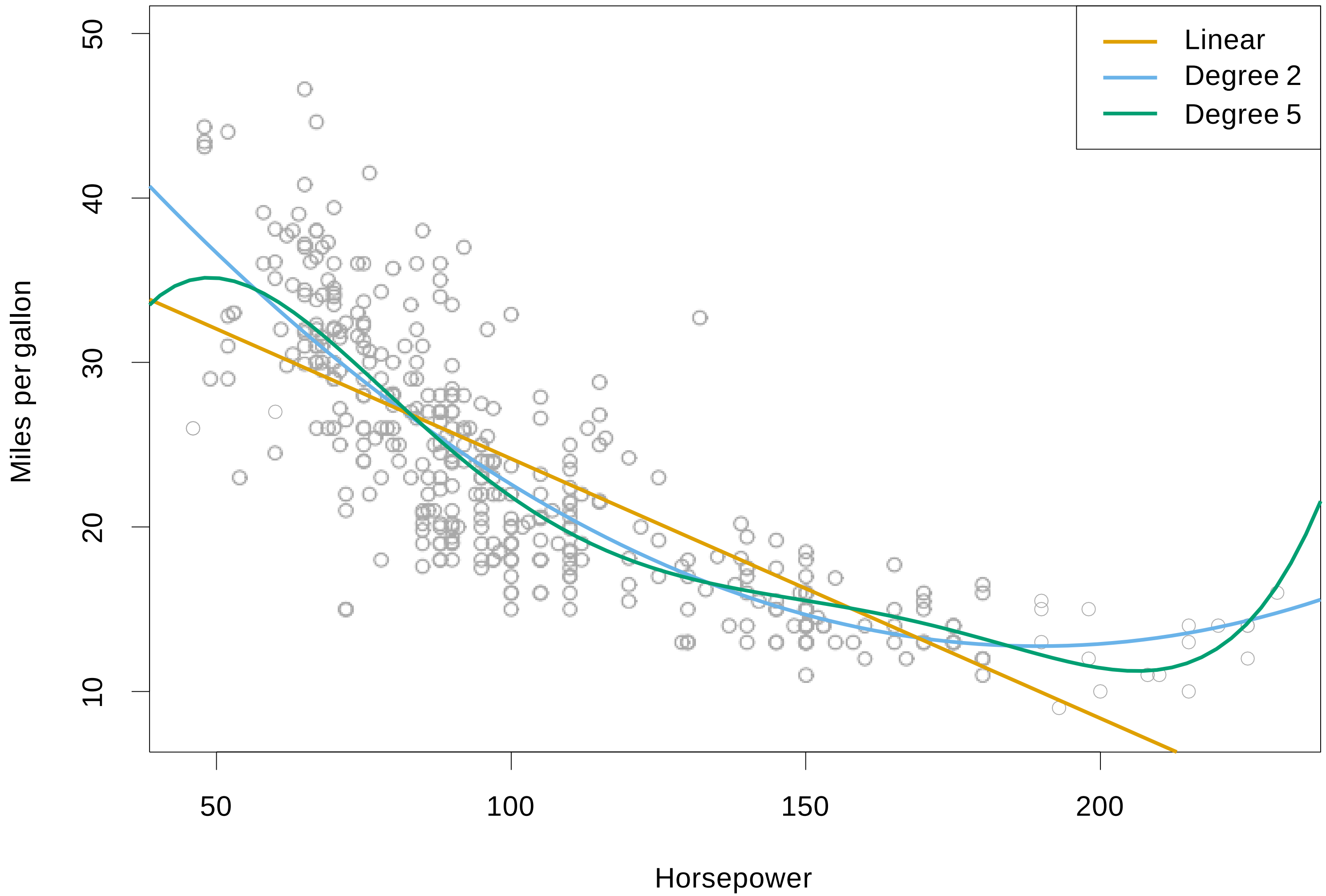
$$
\begin{aligned}
\texttt{balance}_i &\approx \beta_0 + \beta_1 \times \texttt{income}_i + \begin{cases} \beta_2 + \beta_3 \times \texttt{income}_i & \text{if student} \\ 0 & \text{if not student} \end{cases} \\
&= \begin{cases} (\beta_0 + \beta_2) + (\beta_1 + \beta_3) \times \texttt{income}_i & \text{if student} \\ \beta_0 + \beta_1 \times \texttt{income}_i & \text{if not student} \end{cases}
\end{aligned}
$$



Credit data; Left: no interaction between income and student.
Right: with an interaction term between income and student.

Non-linear effects of predictors

polynomial regression on Auto data



Non-linear effects of predictors

The figure suggests that

$$\text{mpg} = \beta_0 + \beta_1 \times \text{horsepower} + \beta_2 \times \text{horsepower}^2 + E$$

may provide a better fit.

	Coefficient	Std. Error	t-statistic	p-value
Intercept	56.9001	1.8004	31.6	< 0.0001
horsepower	-0.4662	0.0311	-15.0	< 0.0001
horsepower^2	0.0012	0.0001	10.1	< 0.0001