Linear Regression

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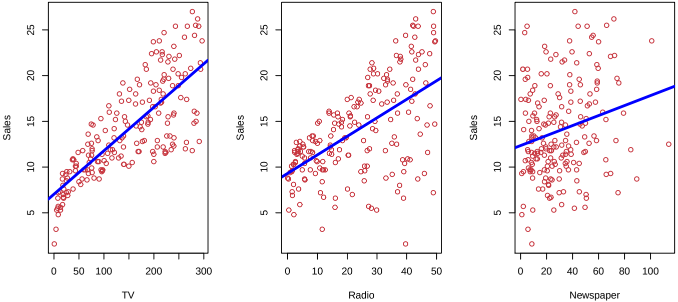
Linear Regression

- **Many of the slides (Marked as T) in this lecture are from Gareth James, Daniella Witten, Trevor Hastie and Robert Tibshirani's book on "An Introduction to Statistical Learning with Applications in R"**

What is Statistical Learning?



Shown are Sales vs TV, Radio and Newspaper, with a blue linear-regression line fit separately to each.

Can we predict Sales using these three?

Perhaps we can do better using a model

$$\texttt{Sales} \approx f(\texttt{TV}, \texttt{Radio}, \texttt{Newspaper})$$

Notation

Here Sales is a *response* or *target* that we wish to predict. We generically refer to the response as Y.
TV is a *feature*, or *input*, or *predictor*; we name it X_1.
Likewise name Radio as X_2, and so on.
We can refer to the *input vector* collectively as

$$X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix}$$

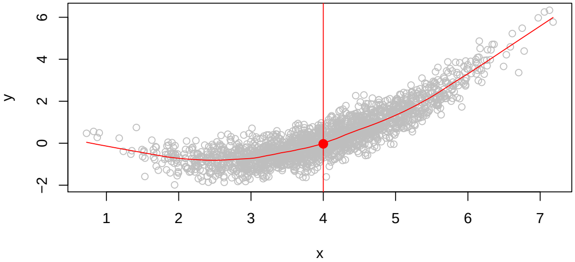
Now we write our model as

$$Y = f(X) + \epsilon$$

where ϵ captures measurement errors and other discrepancies.

What is $f(X)$ good for?

- With a good f we can make predictions of Y at new points $X = x$.
- We can understand which components of $X = (X_1, X_2, \ldots, X_p)$ are important in explaining Y, and which are irrelevant. e.g. `Seniority` and `Years of Education` have a big impact on `Income`, but `Marital Status` typically does not.
- Depending on the complexity of f, we may be able to understand how each component X_j of X affects Y.



Is there an ideal $f(X)$? In particular, what is a good value for $f(X)$ at any selected value of X, say $X = 4$? There can be many Y values at $X = 4$. A good value is

$$f(4) = E(Y|X = 4)$$

$E(Y|X = 4)$ means *expected value* (average) of Y given $X = 4$.

This ideal $f(x) = E(Y|X = x)$ is called the *regression function*.

The regression function $f(x)$

- Is also defined for vector X; e.g.
  $f(x) = f(x_1, x_2, x_3) = E(Y|X_1 = x_1, X_2 = x_2, X_3 = x_3)$

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- Is the *ideal* or *optimal* predictor of Y with regard to mean-squared prediction error: $f(x) = E(Y|X = x)$ is the function that minimizes $E[(Y - g(X))^2|X = x]$ over all functions g at all points $X = x$.

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- $\epsilon = Y - f(x)$ is the *irreducible* error — i.e. even if we knew $f(x)$, we would still make errors in prediction, since at each $X = x$ there is typically a distribution of possible Y values.
- For any estimate $\hat{f}(x)$ of $f(x)$, we have

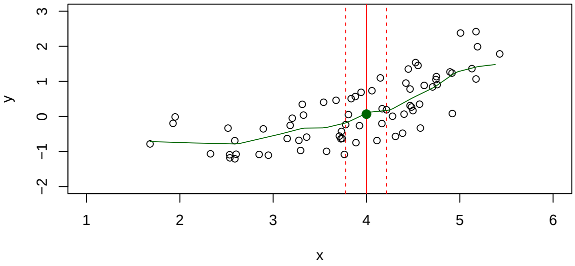
$$E[(Y - \hat{f}(X))^2|X = x] = \underbrace{[f(x) - \hat{f}(x)]^2}_{\textit{Reducible}} + \underbrace{\mathrm{Var}(\epsilon)}_{\textit{Irreducible}}$$

How to estimate f

- Typically we have few if any data points with $X = 4$ exactly.
- So we cannot compute $E(Y|X = x)$!
- Relax the definition and let

$$\hat{f}(x) = \text{Ave}(Y|X \in \mathcal{N}(x))$$

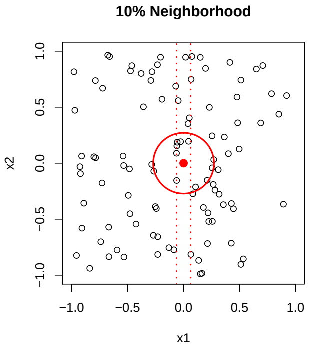
where $\mathcal{N}(x)$ is some *neighborhood* of x.

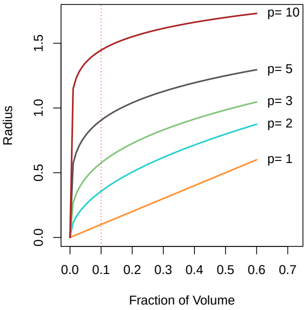


- Nearest neighbor averaging can be pretty good for small p — i.e. $p \leq 4$ and large-ish N.
- We will discuss smoother versions, such as kernel and spline smoothing later in the course.

- Nearest neighbor averaging can be pretty good for small p — i.e. $p \leq 4$ and large-ish N.
- We will discuss smoother versions, such as kernel and spline smoothing later in the course.
- Nearest neighbor methods can be *lousy* when p is large. Reason: the *curse of dimensionality*. Nearest neighbors tend to be far away in high dimensions.
    - We need to get a reasonable fraction of the N values of y_i to average to bring the variance down—e.g. 10%.
    - A 10% neighborhood in high dimensions need no longer be local, so we lose the spirit of estimating $E(Y|X = x)$ by local averaging.

The curse of dimensionality





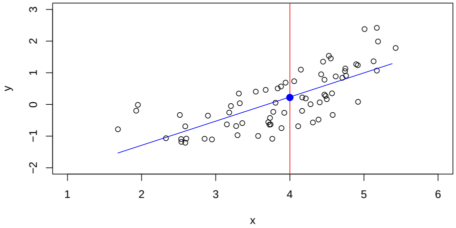
Parametric and structured models

The *linear* model is an important example of a parametric model:

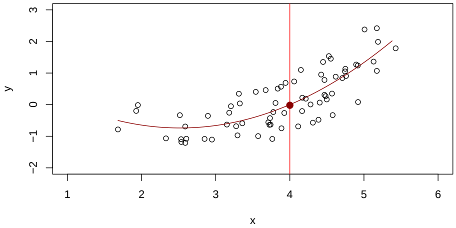
$$f_L(X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots \beta_p X_p.$$

- A linear model is specified in terms of $p + 1$ parameters $\beta_0, \beta_1, \ldots, \beta_p$.
- We estimate the parameters by fitting the model to training data.
- Although it is *almost never correct*, a linear model often serves as a good and interpretable approximation to the unknown true function $f(X)$.

A linear model $\hat{f}_L(X) = \hat{\beta}_0 + \hat{\beta}_1 X$ gives a reasonable fit here



A quadratic model $\hat{f}_Q(X) = \hat{\beta}_0 + \hat{\beta}_1 X + \hat{\beta}_2 X^2$ fits slightly better.



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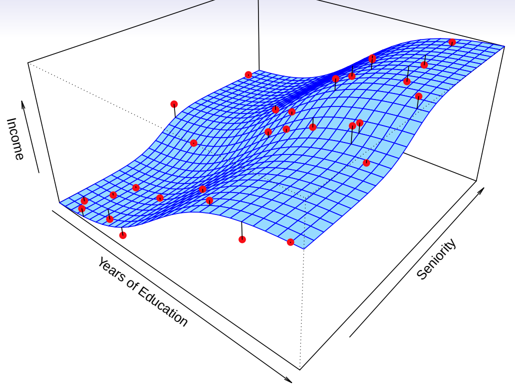
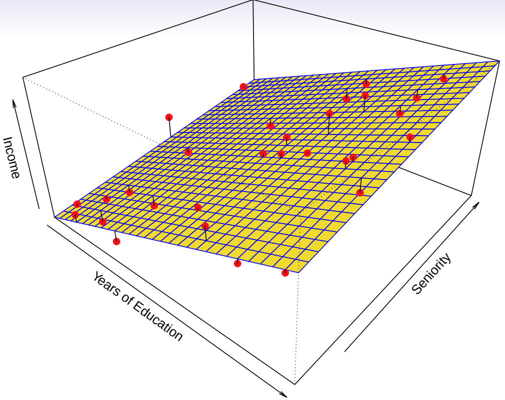


Simulated example. Red points are simulated values for `income` from the model

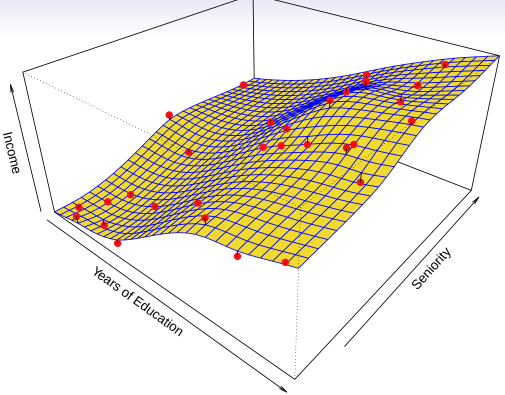
$$\texttt{income} = f(\texttt{education}, \texttt{seniority}) + \epsilon$$

f is the blue surface.



Linear regression model fit to the simulated data.

$$\hat{f}_L(\texttt{education}, \texttt{seniority}) = \hat{\beta}_0 + \hat{\beta}_1 \times \texttt{education} + \hat{\beta}_2 \times \texttt{seniority}$$



More flexible regression model $\hat{f}_S(\texttt{education}, \texttt{seniority})$ fit to the simulated data. Here we use a technique called a *thin-plate spline* to fit a flexible surface. We control the roughness of the fit (chapter 7).

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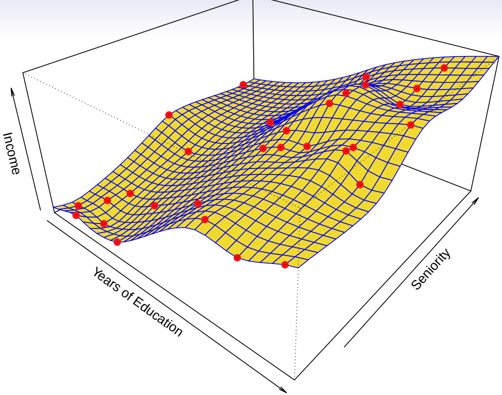

Even more flexible spline regression model $\hat{f}_S(\texttt{education}, \texttt{seniority})$ fit to the simulated data. Here the fitted model makes no errors on the training data! Also known as *overfitting*.

Some trade-offs

- Prediction accuracy versus interpretability.
  — Linear models are easy to interpret; thin-plate splines are not.

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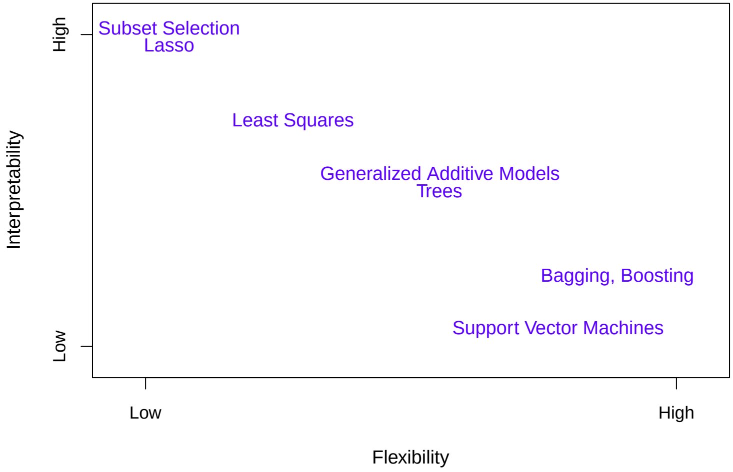
Some trade-offs

- Prediction accuracy versus interpretability.
  — Linear models are easy to interpret; thin-plate splines are not.
- Good fit versus over-fit or under-fit.
  — How do we know when the fit is just right?
- Parsimony versus black-box.
  — We often prefer a simpler model involving fewer variables over a black-box predictor involving them all.



Subset Selection
Lasso
Least Squares
Generalized Additive Models
Trees
Bagging, Boosting
Support Vector Machines
Interpretability
High
Low
Low
High
Flexibility

Estimators, Bias and Variance

- Point Estimation
  - Provides single best prediction of some quantity of interest
  - If $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$ represents *m* independent data points, then point estimator is
    - Any function of the data $\hat{\theta}_m = g(x^{(1)}, x^{(2)}, \dots, x^{(m)})$
  - Good point estimates are close to true θ
- For linear regression
  - For different set of *m* independent data points, we get different model parameters for $\hat{f}(x_0)$
    - Expectation $E[\hat{f}(x_0)]$

Bias and Variance

- Bias$\left[\hat{\theta}_m\right] = E\left(\hat{\theta}_m\right) - \theta$
  - For linear regression
    - Bias$\left[\hat{f}(x)\right] = E\left(\hat{f}(x)\right) - f(x)$
- Variance$\left[\hat{\theta}_m\right] = E\left[\left(\hat{\theta}_m - E\left(\hat{\theta}_m\right)\right)^2\right]$

$$= E\left[\left(\hat{\theta}_m\right)^2\right] - 2\left(E\left(\hat{\theta}_m\right)\right)^2 + \left(E\left(\hat{\theta}_m\right)\right)^2$$

$$= E\left[\left(\hat{\theta}_m\right)^2\right] - \left(E\left(\hat{\theta}_m\right)\right)^2$$

Mean Square Error

- $$E\left[\left(\hat{\theta}_m - \theta\right)^2\right] = E\left[\hat{\theta}_m{}^2 - 2\theta\hat{\theta}_m + \theta^2\right]$$
$$= E\left[\hat{\theta}_m{}^2\right] - 2\theta E\left[\hat{\theta}_m\right] + E[\theta^2]$$
$$= Var\left(\hat{\theta}_m\right) + \left(E\left[\hat{\theta}_m\right]\right)^2 - 2\theta E\left[\hat{\theta}_m\right] + E[\theta^2]$$
$$= Var\left(\hat{\theta}_m\right) + \left(E\left[\hat{\theta}_m\right] - \theta\right)^2$$
$$= Var\left(\hat{\theta}_m\right) + \left[Bias\left(\hat{\theta}_m\right)\right]^2$$

Assessing Model Accuracy

Suppose we fit a model $\hat{f}(x)$ to some training data $\mathsf{Tr} = \{x_i, y_i\}_1^N$, and we wish to see how well it performs.

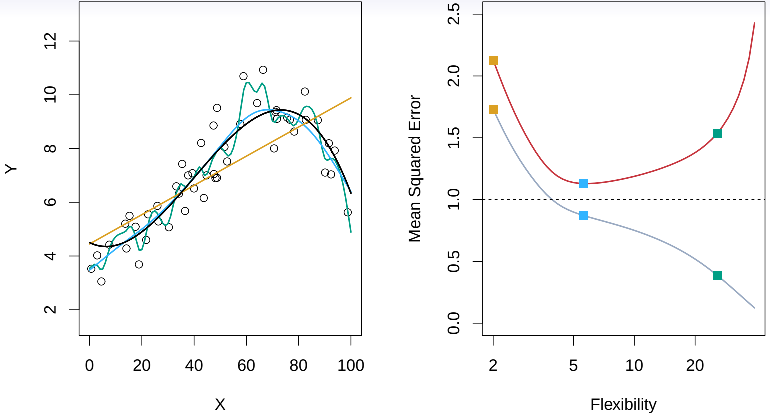
- We could compute the average squared prediction error over Tr:

$$\mathrm{MSE}_{\mathsf{Tr}} = \mathrm{Ave}_{i \in \mathsf{Tr}}[y_i - \hat{f}(x_i)]^2$$

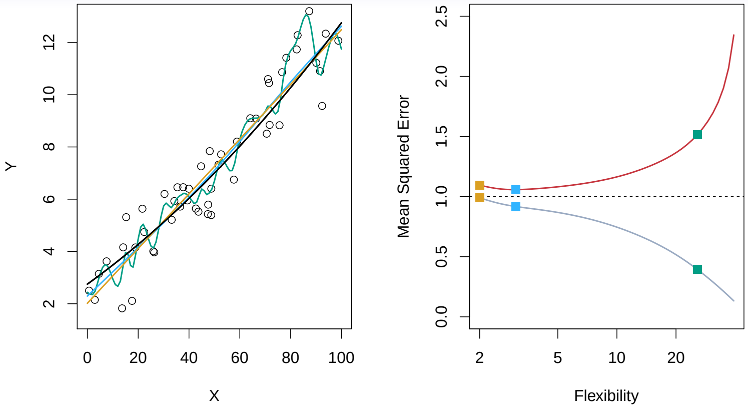
This may be biased toward more overfit models.

- Instead we should, if possible, compute it using fresh *test* data $\mathsf{Te} = \{x_i, y_i\}_1^M$:

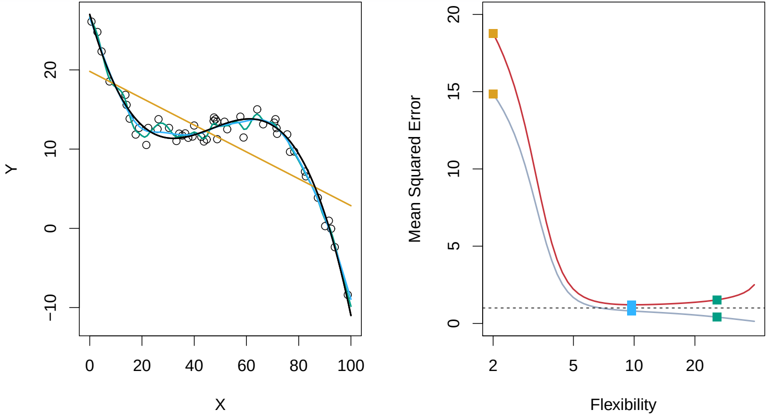
$$\mathrm{MSE}_{\mathsf{Te}} = \mathrm{Ave}_{i \in \mathsf{Te}}[y_i - \hat{f}(x_i)]^2$$



Black curve is truth. Red curve on right is $\mathrm{MSE}_{\mathsf{Te}}$, grey curve is $\mathrm{MSE}_{\mathsf{Tr}}$. Orange, blue and green curves/squares correspond to fits of different flexibility.



Here the truth is smoother, so the smoother fit and linear model do really well.



Here the truth is wiggly and the noise is low, so the more flexible fits do the best.

Bias-Variance Trade-off

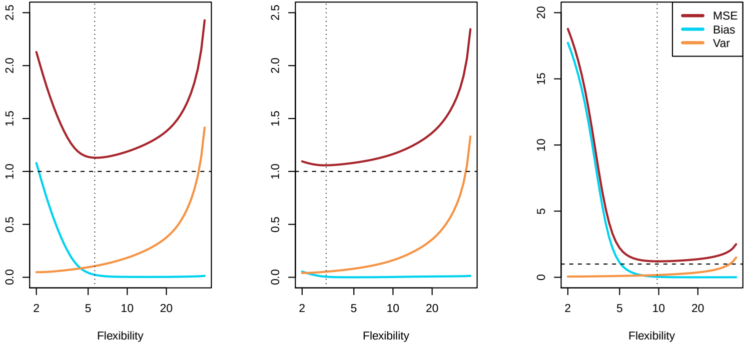
Suppose we have fit a model $\hat{f}(x)$ to some training data Tr, and let (x_0, y_0) be a test observation drawn from the population. If the true model is $Y = f(X) + \epsilon$ (with $f(x) = E(Y|X = x)$), then

$$E\left(y_0 - \hat{f}(x_0)\right)^2 = \text{Var}(\hat{f}(x_0)) + [\text{Bias}(\hat{f}(x_0))]^2 + \text{Var}(\epsilon).$$

The expectation averages over the variability of y_0 as well as the variability in Tr. Note that $\text{Bias}(\hat{f}(x_0))] = E[\hat{f}(x_0)] - f(x_0)$.

Typically as the *flexibility* of $\hat{f}$ increases, its variance increases, and its bias decreases. So choosing the flexibility based on average test error amounts to a *bias-variance trade-off.*

Bias-variance trade-off for the three examples



Linear regression

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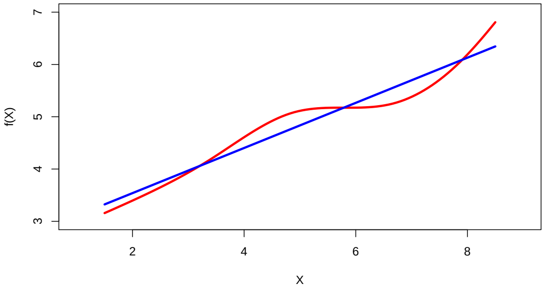
- True regression functions are never linear!



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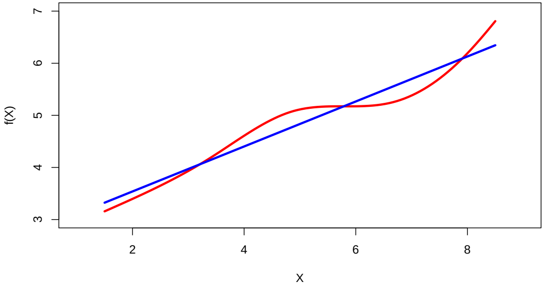


- although it may seem overly simplistic, linear regression is extremely useful both conceptually and practically.

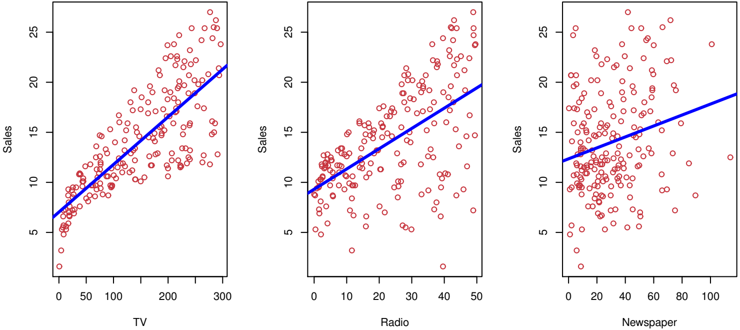
Linear regression for the advertising data

Consider the advertising data shown on the next slide.

Questions we might ask:

- Is there a relationship between advertising budget and sales?
- How strong is the relationship between advertising budget and sales?
- Which media contribute to sales?
- How accurately can we predict future sales?
- Is the relationship linear?
- Is there synergy among the advertising media?

Advertising data



Simple linear regression using a single predictor X.

- We assume a model

$$Y = \beta_0 + \beta_1 X + \epsilon,$$

where β_0 and β_1 are two unknown constants that represent the *intercept* and *slope*, also known as *coefficients* or *parameters*, and ϵ is the error term.

- Given some estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ for the model coefficients, we predict future sales using

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

where $\hat{y}$ indicates a prediction of Y on the basis of $X = x$. The *hat* symbol denotes an estimated value.

Estimation of the parameters by least squares

- Let $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ be the prediction for Y based on the ith value of X. Then $e_i = y_i - \hat{y}_i$ represents the ith *residual*

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- We define the *residual sum of squares* (RSS) as

$$\mathrm{RSS} = e_1^2 + e_2^2 + \cdots + e_n^2,$$

or equivalently as

$$\mathrm{RSS} = (y_1 - \hat{\beta}_0 - \hat{\beta}_1 x_1)^2 + (y_2 - \hat{\beta}_0 - \hat{\beta}_1 x_2)^2 + \ldots + (y_n - \hat{\beta}_0 - \hat{\beta}_1 x_n)^2.$$

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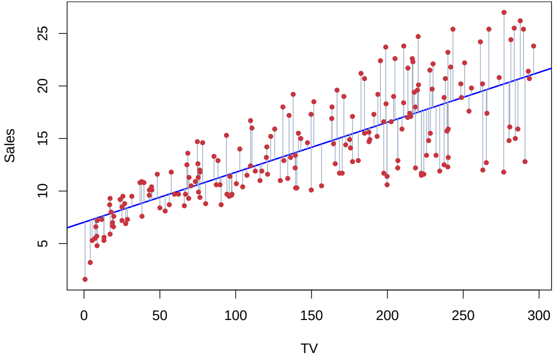
- The least squares approach chooses $\hat{\beta}_0$ and $\hat{\beta}_1$ to minimize the RSS. The minimizing values can be shown to be

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

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

where $\bar{y} \equiv \frac{1}{n} \sum_{i=1}^{n} y_i$ and $\bar{x} \equiv \frac{1}{n} \sum_{i=1}^{n} x_i$ are the sample means.

Example: advertising data



The least squares fit for the regression of sales onto TV.
In this case a linear fit captures the essence of the relationship, although it is somewhat deficient in the left of the plot.

Properties of the least square estimators

- **We assumed that**
  - **The term $Y_i = \beta_0 + \beta_1 x_i + \epsilon_i$ is a random variable**
  - **The error ϵ_i has mean 0 and constant variance σ^2**
  - $\epsilon_1, \epsilon_2, \ldots, \epsilon_n$ **are independent at each run**
- **Since x_i remains fixed, the estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ depends only on $Y_1, Y_2, \ldots, Y_n$.**
- **Considering $Y_1, Y_2, \ldots, Y_n$ to be idependent of each other**
  - **Mean** $\mu_{Y|x_i} = \beta_0 + \beta_1 x_i$
  - **Variance** $\sigma^2_{Y|x_i} = \sigma^2$

Mean and Variance of Estimators

- **Let** B_0 **and** B_1 **denote the random variable of the coefficients**
- **The estimator** $B_1 = \frac{\sum_{i=1}^{n}(x_1 - \overline{x})(Y_i - \overline{Y})}{\sum_{i=1}^{n}(x_i - \overline{x})^2} = \frac{\sum_{i=1}^{n}(x_i - \overline{x})Y_i}{\sum_{i=1}^{n}(x_i - \overline{x})^2}$
- $= \sum_{i=1}^{n} c_i Y_i$ **where** $c_i = \frac{x_i - \overline{x}}{\sum_{i=1}^{n}(x_i - \overline{x})^2}$
- $E[B_1] = \mu_{B_1} = \sum_{i=1}^{n} c_i E[Y_i] = \frac{\sum_{i=1}^{n}(x_1 - \overline{x})(\beta_0 + \beta_1 x_i)}{\sum_{i=1}^{n}(x_i - \overline{x})^2} = \beta_1$
- **Variance**$(B_1) = \sigma_{B_1}^2 = \sum_{i=1}^{n} c_1^2 Var(Y_i) = \frac{\sum_{i=1}^{n}(x_i - \overline{x})^2 \sigma_{Y_i}^2}{\left[\sum_{i=1}^{n}(x_i - \overline{x})^2\right]^2} = \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \overline{x})^2}$
- **it can be shown similarly that** $\mu_{B_0} = \beta_0$ **and** $\sigma_{B_0}^2 = \frac{\sum_{i=1}^{n} x_1^2}{n\sum_{i=1}^{n}(x_i - \overline{x})^2}$

Assessing the Accuracy of the Coefficient Estimates

- The standard error of an estimator reflects how it varies under repeated sampling. We have

$$\mathrm{SE}(\hat\beta_1)^2 = \frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2}, \quad \mathrm{SE}(\hat\beta_0)^2 = \sigma^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2}\right],$$

where $\sigma^2 = \mathrm{Var}(\epsilon)$

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where $\sigma^2 = \mathrm{Var}(\epsilon)$

- These standard errors can be used to compute *confidence intervals*. A 95% confidence interval is defined as a range of values such that with 95% probability, the range will contain the true unknown value of the parameter. It has the form

$$\hat{\beta}_1 \pm 2 \cdot \mathrm{SE}(\hat{\beta}_1).$$

Confidence intervals — continued

That is, there is approximately a 95% chance that the interval

$$\left[\hat{\beta}_1 - 2 \cdot \mathrm{SE}(\hat{\beta}_1),\ \hat{\beta}_1 + 2 \cdot \mathrm{SE}(\hat{\beta}_1)\right]$$

will contain the true value of β_1 (under a scenario where we got repeated samples like the present sample)

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For the advertising data, the 95% confidence interval for β_1 is $[0.042, 0.053]$

Hypothesis testing

- Standard errors can also be used to perform *hypothesis tests* on the coefficients. The most common hypothesis test involves testing the *null hypothesis* of

$$H_0: \quad \text{There is no relationship between } X \text{ and } Y$$

versus the *alternative hypothesis*

$$H_A: \quad \text{There is some relationship between } X \text{ and } Y.$$

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  versus the *alternative hypothesis*

  H_A : There is some relationship between X and Y.

- Mathematically, this corresponds to testing

$$H_0 : \beta_1 = 0$$

versus

$$H_A : \beta_1 \neq 0,$$

since if $\beta_1 = 0$ then the model reduces to $Y = \beta_0 + \epsilon$, and X is not associated with Y.

T

Hypothesis testing — continued

- To test the null hypothesis, we compute a *t-statistic*, given by

$$t = \frac{\hat{\beta}_1 - 0}{\mathrm{SE}(\hat{\beta}_1)},$$

- This will have a t-distribution with $n - 2$ degrees of freedom, assuming $\beta_1 = 0$.
- Using statistical software, it is easy to compute the probability of observing any value equal to $|t|$ or larger. We call this probability the *p-value*.

Results for the advertising data

	Coefficient	Std. Error	t-statistic	p-value
`Intercept`	7.0325	0.4578	15.36	< 0.0001
`TV`	0.0475	0.0027	17.67	< 0.0001

Assessing the Overall Accuracy of the Model

- We compute the *Residual Standard Error*

$$\mathrm{RSE} = \sqrt{\frac{1}{n-2}\mathrm{RSS}} = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2},$$

where the *residual sum-of-squares* is $RSS = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$.

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$$R^2 = \frac{\mathrm{TSS} - \mathrm{RSS}}{\mathrm{TSS}} = 1 - \frac{\mathrm{RSS}}{\mathrm{TSS}}$$

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  where $\mathrm{TSS} = \sum_{i=1}^{n}(y_i - \bar{y})^2$ is the *total sum of squares*.
- It can be shown that in this simple linear regression setting that $R^2 = r^2$, where r is the correlation between X and Y:

$$r = \frac{\sum_{i=1}^{n}(x_i - \overline{x})(y_i - \overline{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \overline{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \overline{y})^2}}.$$

Advertising data results

Quantity	Value
Residual Standard Error	3.26
R^2	0.612
F-statistic	312.1

Multiple Linear Regression

- 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

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

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.

The woes of (interpreting) regression coefficients

"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!

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- 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?

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- $Y =$ number of tackles by a football player in a season; W and H are his weight and height. Fitted regression model is $\hat{Y} = b_0 + .50W - .10H$. How do we interpret $\hat{\beta}_2 < 0$?

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Estimation and Prediction for Multiple Regression

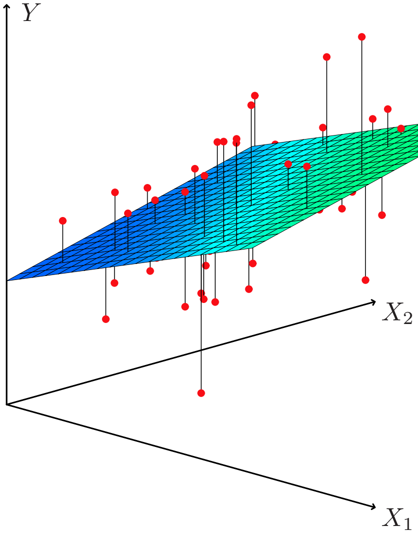
- Given estimates $\hat{\beta}_0, \hat{\beta}_1, \ldots \hat{\beta}_p$, we can make predictions using the formula

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

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

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

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.



Y
X_2
X_1

T

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

Correlations:

	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

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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?

For the first question, we can use the F-statistic

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

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

Deciding on the 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.

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Deciding on the 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.

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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)*.

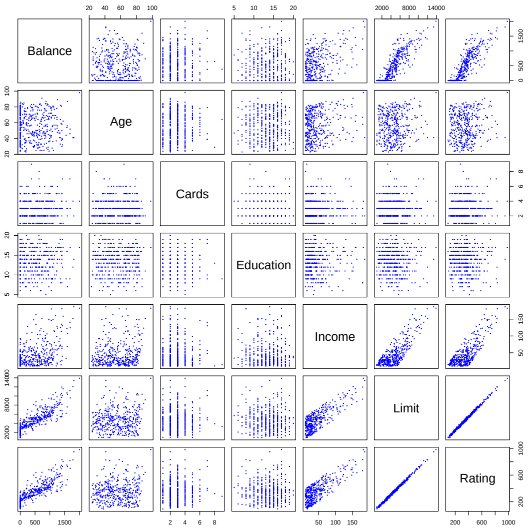
Other Considerations in the Regression Model

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:

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

Intrepretation?

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

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

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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

Extensions of the Linear Model

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

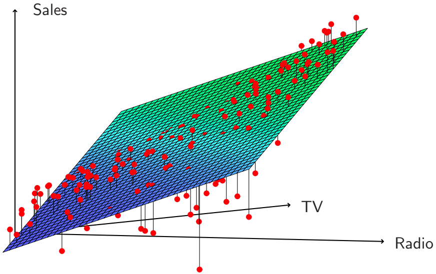
$$\widehat{\texttt{sales}} = \beta_0 + \beta_1 \times \texttt{TV} + \beta_2 \times \texttt{radio} + \beta_3 \times \texttt{newspaper}$$

  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

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

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 $(\hat{\beta}_1 + \hat{\beta}_3 \times \texttt{radio}) \times 1000 = 19 + 1.1 \times \texttt{radio}$ units.
- An increase in radio advertising of $\$1,000$ will be associated with an increase in sales of $(\hat{\beta}_2 + \hat{\beta}_3 \times \texttt{TV}) \times 1000 = 29 + 1.1 \times \texttt{TV}$ units.

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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.

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Hierarchy — continued

- 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.

T

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

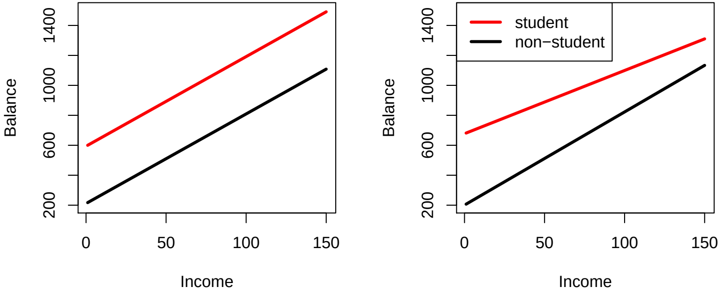
$$
\begin{aligned}
\texttt{balance}_i &\approx \beta_0 + \beta_1 \times \texttt{income}_i + \begin{cases} \beta_2 & \text{if } i\text{th person is a student} \\ 0 & \text{if } i\text{th person is not a student} \end{cases} \\
&= \beta_1 \times \texttt{income}_i + \begin{cases} \beta_0 + \beta_2 & \text{if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

T

With interactions, it takes the form

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

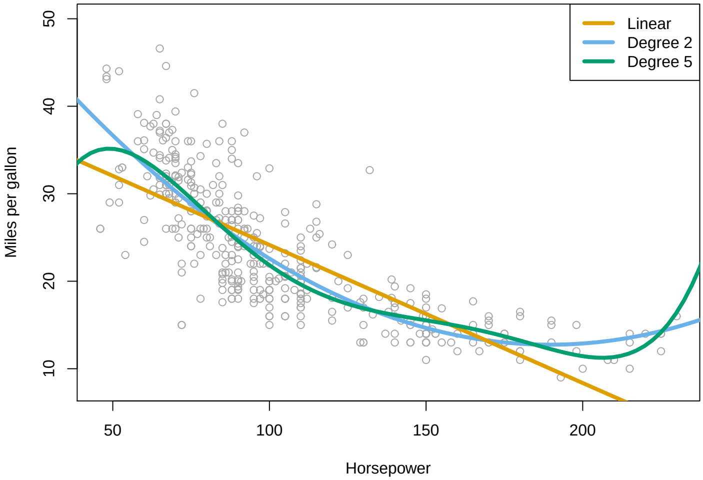
$$= \begin{cases} (\beta_0 + \beta_2) + (\beta_1 + \beta_3) \times \texttt{income}_i & \text{if student} \\ \beta_0 + \beta_1 \times \texttt{income}_i & \text{if not student} \end{cases}$$



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



The figure suggests that

$$\texttt{mpg} = \beta_0 + \beta_1 \times \texttt{horsepower} + \beta_2 \times \texttt{horsepower}^2 + \epsilon$$

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
$\texttt{horsepower}^2$	0.0012	0.0001	10.1	< 0.0001

References

- "An Introduction to Statistical Learning with Applications in R" by Gareth James, Daniella Witten, Trevor Hastie and Robert Tibshirani
- "Probability and Statistics for Engineers and Scientists" by Walpole Meyers, Meyers and Ye
- "Statistics for Management" by Levin and Rubin
- Useful resource on Regression Using Excel, "https://www.ablebits.com/office-addins-blog/2018/08/01/linear-regression-analysis-excel/"