Lecture 7: Linear Regression (continued)

Reading: Chapter 3

STATS 202: Data mining and analysis

October 07, 2019

Potential issues in linear regression

1. Interactions between predictors
2. Non-linear relationships
3. Correlation of error terms
4. Non-constant variance of error (heteroskedasticity).
5. Outliers
6. High leverage points
7. Collinearity

Correlation of error terms

We assumed that the errors for each sample are independent:

$$y_i = f(x_i) + \varepsilon_i \quad ; \quad \varepsilon_i \sim \mathcal{N}(0, \sigma) \text{ i.i.d.}$$

What if this assumption breaks down?

The main effect is that this invalidates any assertions about Standard Errors, confidence intervals, and hypothesis tests:

Example: Suppose that by accident, we double the data (we use each sample twice). Then, the standard errors would be artificially smaller by a factor of $\sqrt{2}$, due to the square-root law.

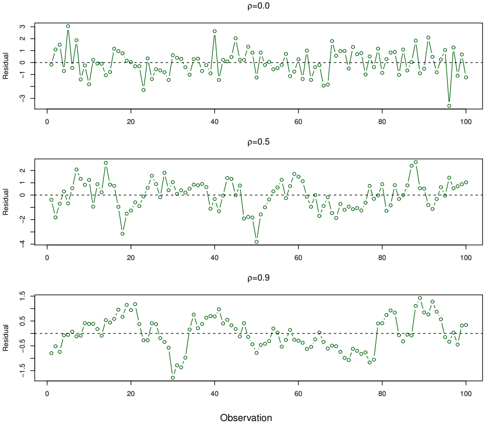
Correlation of error terms

When could this happen in real life:

- **Time series:** Each sample corresponds to a different point in time. The errors for samples that are close in time are correlated.
- **Spatial data:** Each sample corresponds to a different location in space.
- **Predicting height from weight at birth:** Suppose some of the subjects in the study are in the same family, their shared environment could make them deviate from $f(x)$ in similar ways.

Correlation of error terms

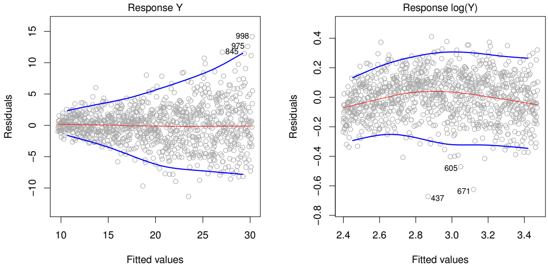
Simulations of time series with increasing correlations between ε_i.



Non-constant variance of error (heteroskedasticity)

For example, the variance of the error depends on the input.

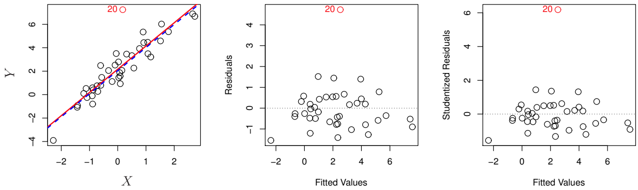
To diagnose this, we can plot residuals vs. fitted values:



Solution: If the trend in variance is relatively simple, we can transform the response using a logarithm, for example.

Outliers

Outliers are points with very high errors.



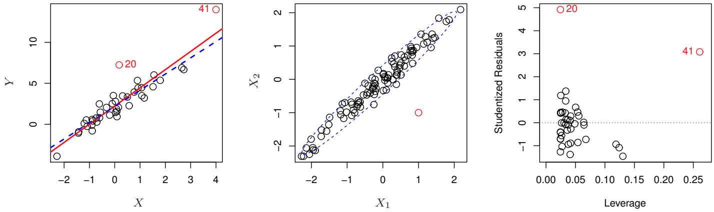
While they may or may not affect the fit, they might affect our assessment of model quality.

Possible solutions:

- If we believe an outlier is due to an error in data collection, we can remove it.
- An outlier might be evidence of a missing predictor, or the need to specify a more complex model.

High leverage points

High leverage points are observations with unusual input values. They can have an outsized effect on the fit $\hat{\beta}$!



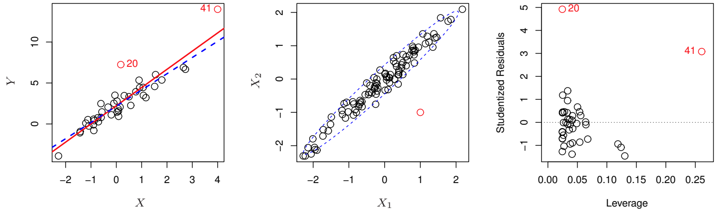
Quantified with the **leverage statistic** or **self influence**:

$$h_{ii} = \frac{\partial \hat{y}_i}{\partial y_i} = (\underbrace{\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T}_{\text{Hat matrix}})_{i,i} \in [1/n, 1].$$

Hat matrix satisfies $\hat{y} = \mathbf{X}\hat{\beta} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T y = \mathbf{H}y$

Studentized residuals

- The residual $\hat{\epsilon}_i = y_i - \hat{y}_i$ is an estimate for the noise $\epsilon_i = y_i - f(x_i)$.
- The standard error of $\hat{\epsilon}_i$ is $\sigma\sqrt{1 - h_{ii}}$.
- A **studentized residual** is $\hat{\epsilon}_i$ divided by its standard error.
- If the model is correct, it follows a Student-t distribution with $n - p - 2$ degrees of freedom.

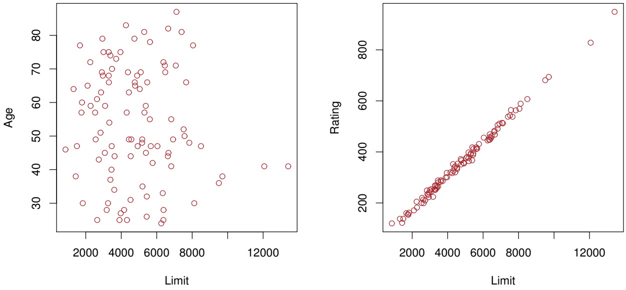


Collinearity

Two predictors are collinear if they are highly correlated:

$$\texttt{limit} \approx a \times \texttt{rating} + b$$

i.e. if one variable is approximately a linear function of the other. In that case they contain approximately the same information.

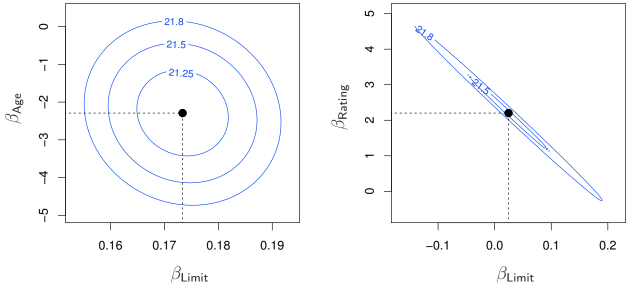


Collinearity

Problem: Coefficient estimates become less certain and more variable (as training data changes). Consider the extreme case of using two identical predictors `limit`:

$$\begin{aligned}\texttt{balance} &= \beta_0 + \beta_1 \times \texttt{limit} + \beta_2 \times \texttt{limit} \\ &= \beta_0 + (\beta_1 + 100) \times \texttt{limit} + (\beta_2 - 100) \times \texttt{limit}\end{aligned}$$

The fit $(\hat\beta_0, \hat\beta_1, \hat\beta_2)$ is just as good as $(\hat\beta_0, \hat\beta_1 + 100, \hat\beta_2 - 100)$.



Collinearity

If 2 variables are collinear, we can easily diagnose this using their correlation.

A group of q variables is **multilinear** if one variable is approximately a linear function of the other variables. Pairwise correlations may not reveal multilinear variables.

The Variance Inflation Factor (VIF) measures how linearly predictable a variable is from the other variables:

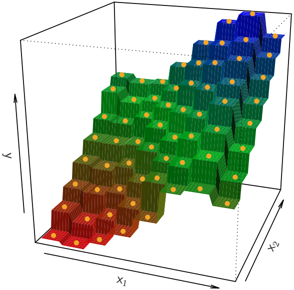
$$VIF(\hat{\beta}_j) = \frac{1}{1 - R^2_{X_j|X_{-j}}},$$

where $R^2_{X_j|X_{-j}}$ is the R^2 statistic for Multiple Linear regression of the predictor X_j onto the remaining predictors.

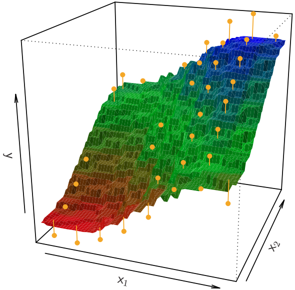
Comparing Linear Regression to K-nearest neighbors

Linear regression: prototypical parametric method.
KNN regression: prototypical nonparametric method.

$$\hat{f}(x) = \frac{1}{K} \sum_{x_i \in N_K(x)} y_i$$



$K = 1$



$K = 9$

Comparing Linear Regression to K-nearest neighbors

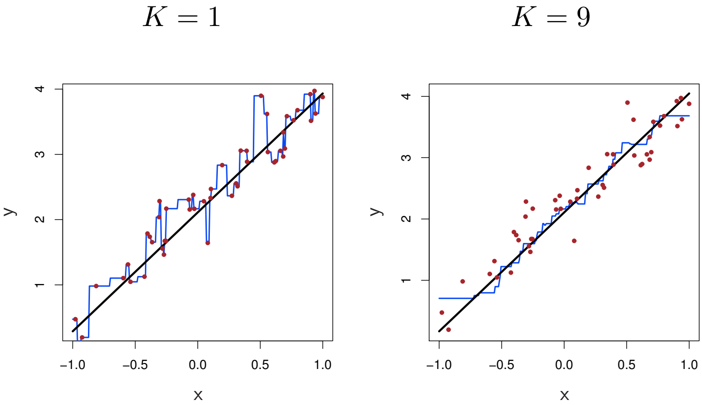
Linear regression: prototypical parametric method.

KNN regression: prototypical nonparametric method.

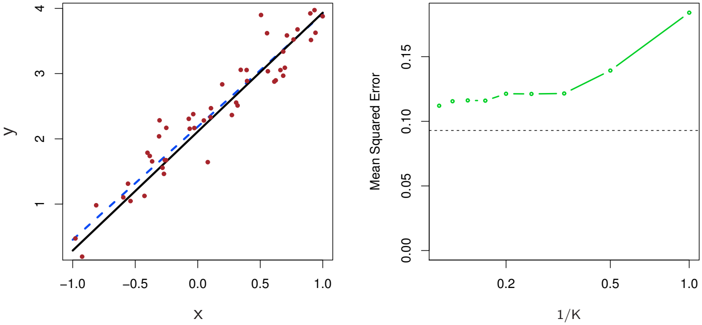
Long story short:

- KNN is only better when the function f is not linear.
- When n is not much larger than p, even if f is nonlinear, Linear Regression can outperform KNN. KNN has smaller bias, but this comes at a price of higher variance.

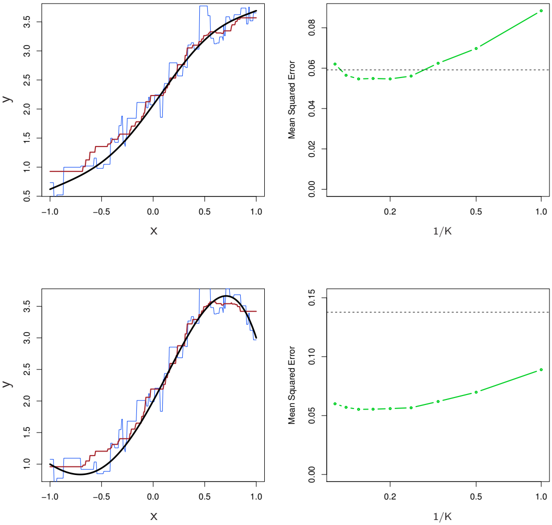
KNN estimates for a simulation from a linear model



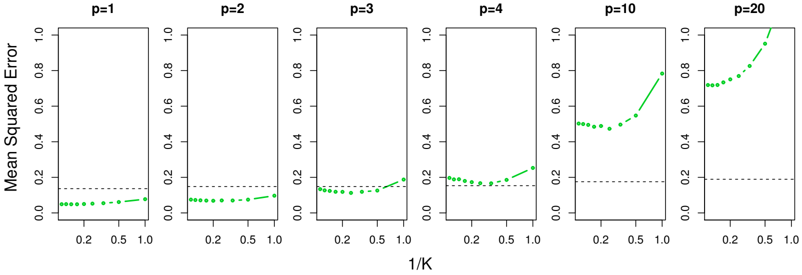
Linear models dominate KNN when true model linear



Increasing deviations from linearity



When the number of predictors is large, Linear Regression can dominate KNN



When p sufficiently large, the nearest neighbors are not especially near, and KNN accuracy can break down. This is known as the *curse of dimensionality*.

Next time: Classification

Supervised learning with a **qualitative or categorical** response.

Just as common, if not more common than regression:

- *Medical diagnosis:* Given the symptoms a patient shows, predict which of 3 conditions they are attributed to.
- *Online banking:* Determine whether a transaction is fraudulent or not, on the basis of the IP address, client's history, etc.
- *Web searching:* Based on a user's history, location, and the string of a web search, predict which link a person is likely to click.
- *Online advertising:* Predict whether a user will click on an ad or not.