Polynomial Regression

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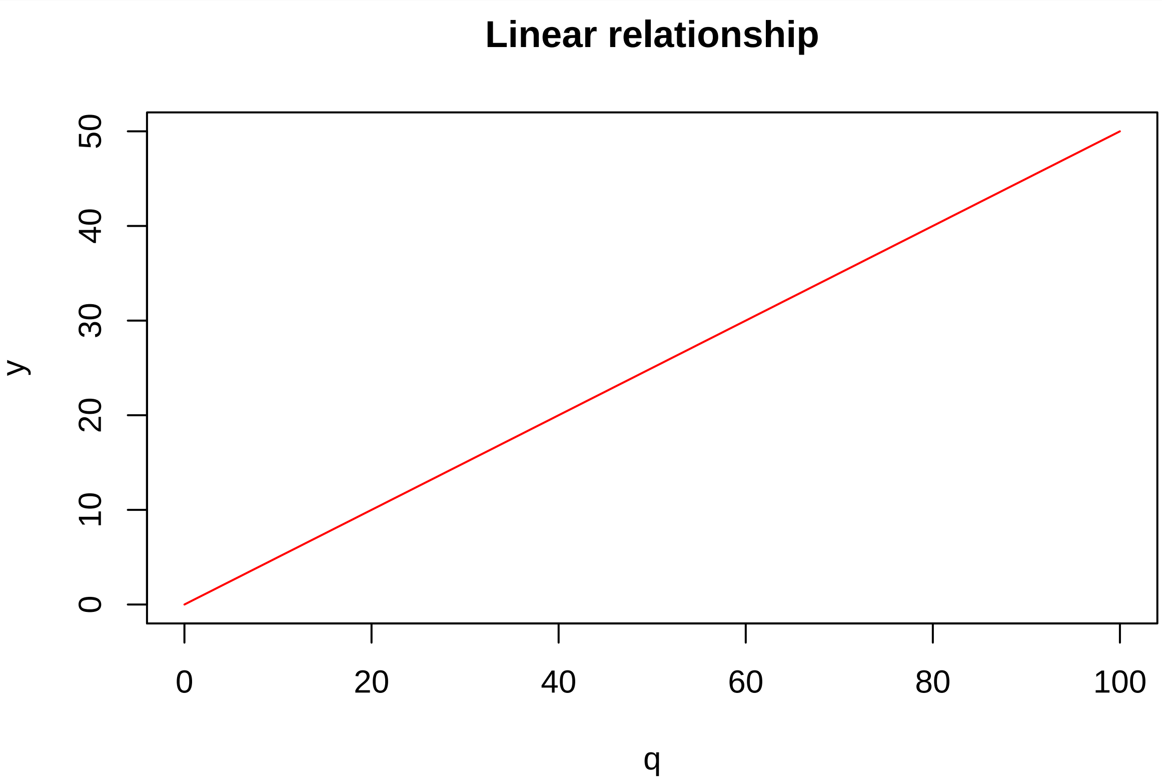
[http://datascienceplus.com/fitting-polynomial-regression-r/]

Intro

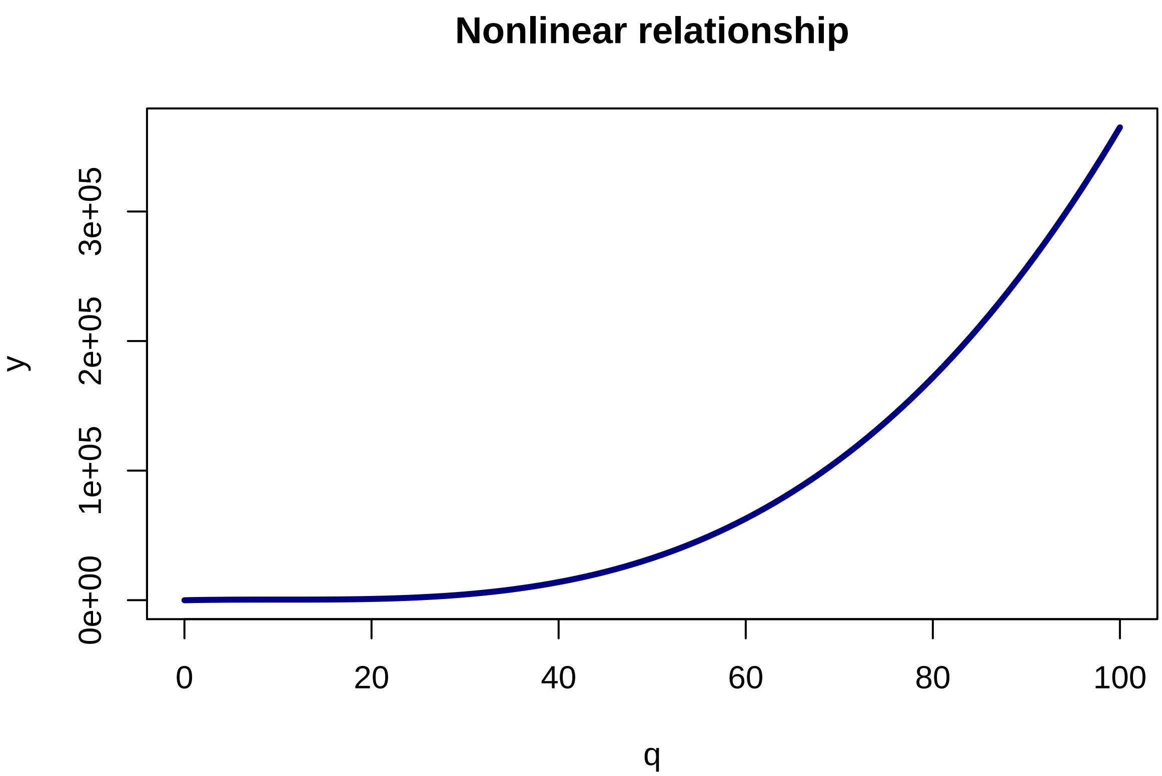
A linear relationship between two variables x and y is one of the most common, effective and easy assumptions to make when trying to figure out their relationship. Sometimes however, the true underlying relationship is more complex than that, and this is when polynomial regression comes in to help. Let see an example from economics: Suppose you would like to buy a certain quantity q of a certain product. If the unit price is p, then you would pay a total amount y. This is a typical example of a linear relationship. Total price and quantity are directly proportional. To plot it we would write something like this:

```
p <- 0.5
q <- seq(0,100,1)
y <- p*q
plot(q,y,type='l',col='red',main='Linear relationship')
```



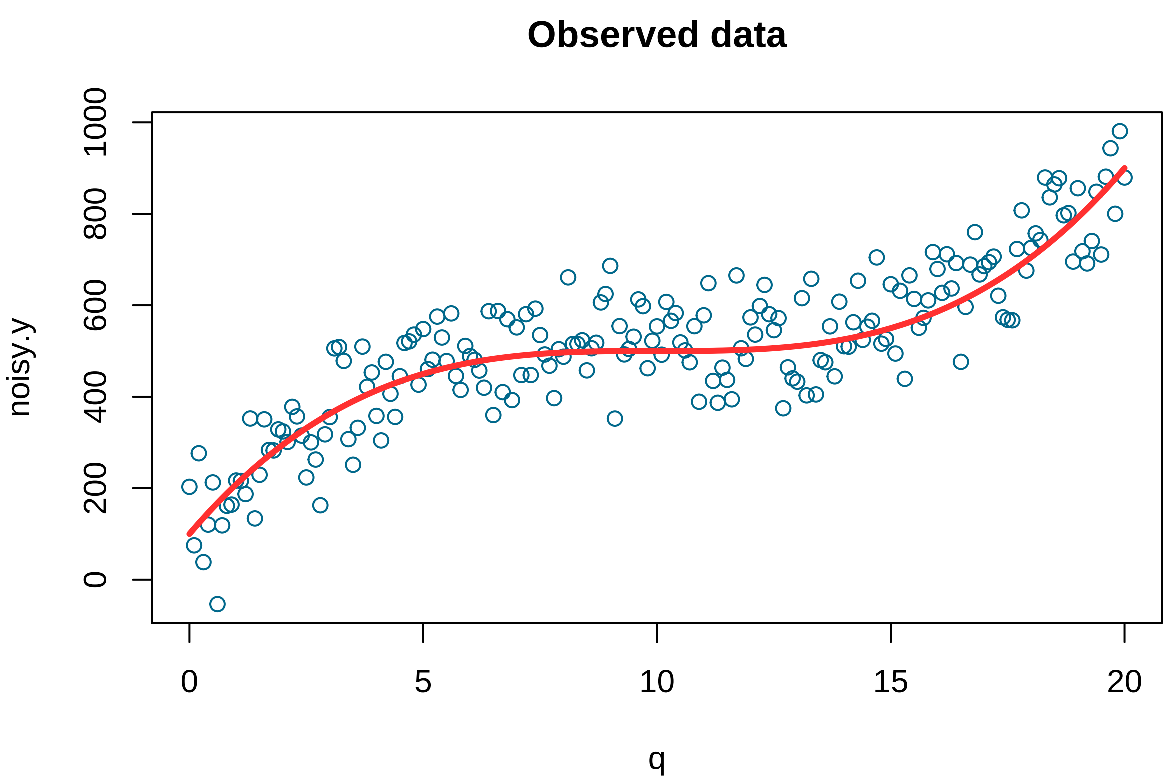
Now, this is a good approximation of the true relationship between y and q, however when buying and selling we might want to consider some other relevant information, like: Buying significant quantities it is likely that we can ask and get a discount, or buying more and more of a certain good we might be pushing the price up. This can lead to a scenario like this one where the total cost is no longer a linear function of the quantity:

```
y <- 450 + p*(q-10)^3
plot(q,y,type='l',col='navy',main='Nonlinear relationship',lwd=3)
```



With polynomial regression we can fit models of order `n > 1` to the data and try to model nonlinear relationships.

Generate Data:



The simulated datapoints are the blue dots while the red line is the signal (signal is a technical term that is often used to indicate the general trend we are interested in detecting).

Our model should be something like this: $y = a * q + b * q2 + c * q3 + cost$

Let's fit it using R. When fitting polynomials you can either

```
model <- lm(noisy.y ~ poly(q,3)) # or...
# model <- lm(noisy.y ~ x + I(X^2) + I(X^3))
```

However, note that q, I(q^2) and I(q^3) will be correlated and correlated variables can cause problems. The use of poly() lets you avoid this by producing orthogonal polynomials, therefore I'm going to use the first option.

```
summary(model)
```

```
##
## Call:
## lm(formula = noisy.y ~ poly(q, 3))
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -212.326  -51.186    4.276   61.485  165.960
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  513.615      5.602   91.69   <2e-16 ***
## poly(q, 3)1 2075.899     79.422   26.14   <2e-16 ***
## poly(q, 3)2 -108.004     79.422   -1.36    0.175
## poly(q, 3)3  864.025     79.422   10.88   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 79.42 on 197 degrees of freedom
## Multiple R-squared:  0.8031, Adjusted R-squared:  0.8001
## F-statistic: 267.8 on 3 and 197 DF,  p-value: < 2.2e-16
```

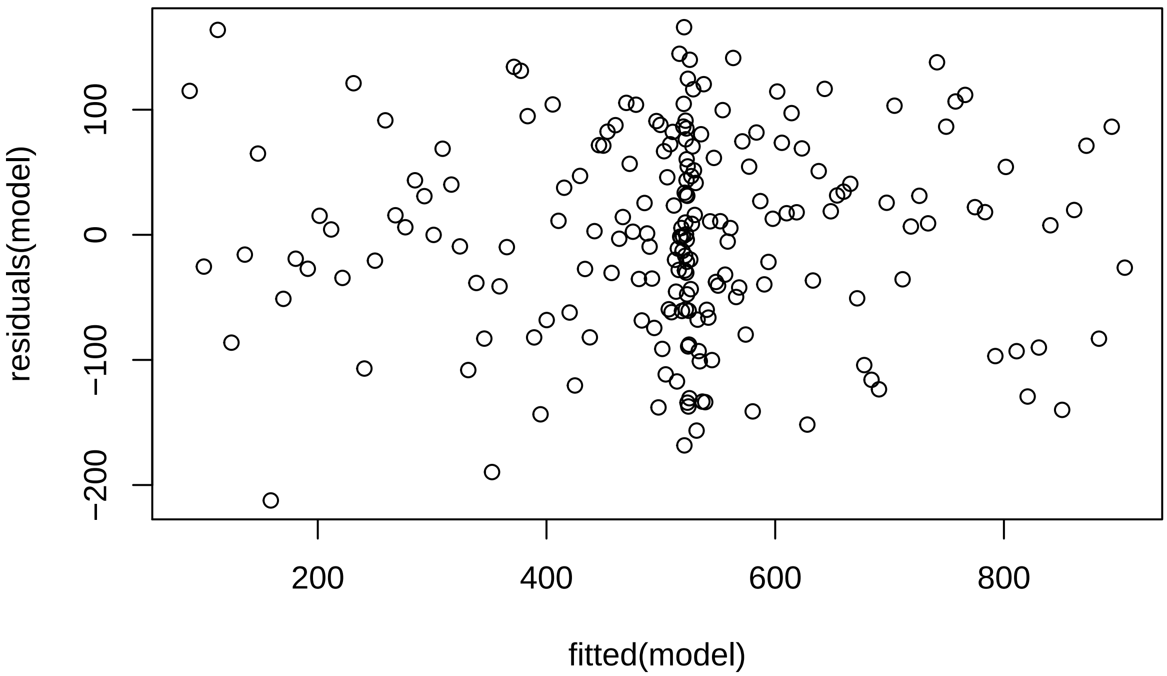
By using the confint() function we can obtain the confidence intervals of the parameters of our model. Confidence intervals for model parameters:

```
confint(model, level=0.95)
```

```
##                 2.5 %     97.5 %
## (Intercept)  502.5676  524.66261
## poly(q, 3)1 1919.2739 2232.52494
## poly(q, 3)2 -264.6292   48.62188
## poly(q, 3)3  707.3999 1020.65097
```

Plot of fitted vs residuals. No clear pattern should show in the residual plot if the model is a good fit

```
plot(fitted(model),residuals(model))
```

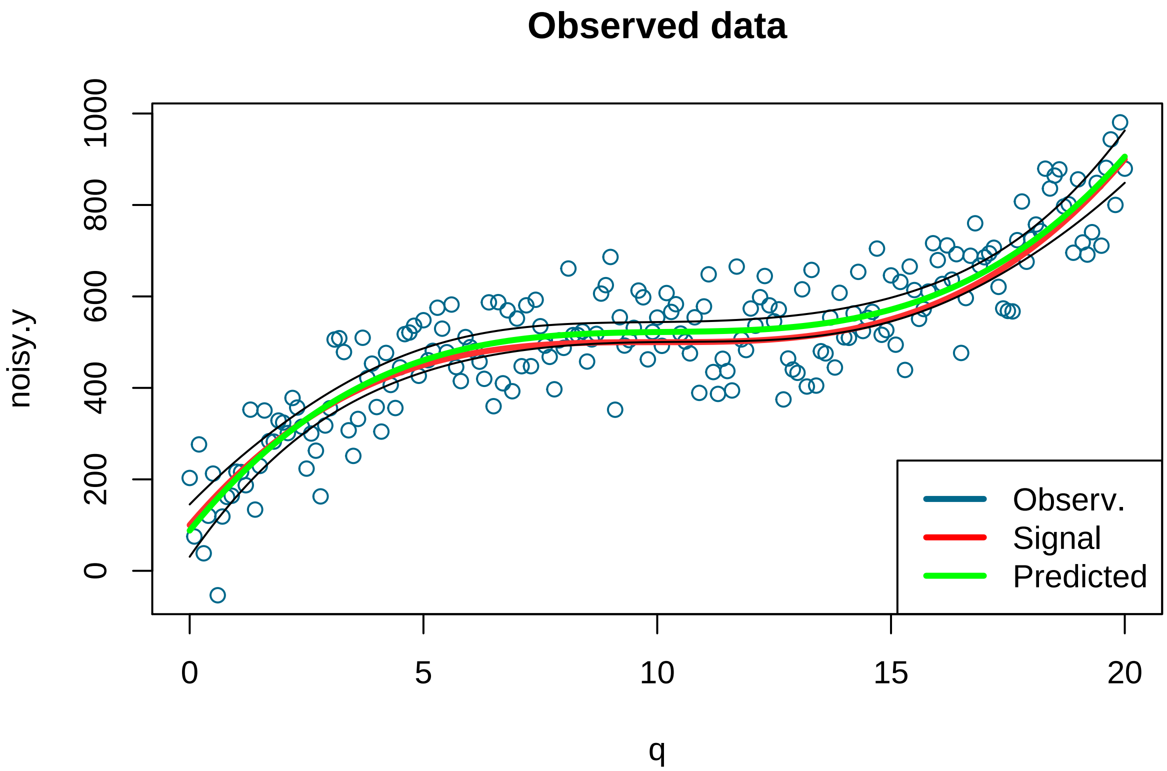


Overall the model seems a good fit as the R squared of 0.8 indicates. The coefficients of the first and third order terms are statistically significant as we expected. Now we can use the predict() function to get the fitted values and the confidence intervals in order to plot everything against our data.

Predicted values and confidence intervals:

```
predicted.intervals <- predict(model,data.frame(x=q),interval='confidence',
                                level=0.99)
```

```
plot(q,noisy.y,col='deepskyblue4',xlab='q',main='Observed data')
lines(q,y,col='firebrick1',lwd=3)
lines(q,predicted.intervals[,1],col='green',lwd=3)
lines(q,predicted.intervals[,2],col='black',lwd=1)
lines(q,predicted.intervals[,3],col='black',lwd=1)
legend("bottomright",c("Observ.","Signal","Predicted"),
       col=c("deepskyblue4","red","green"), lwd=3)
```



We can see that our model did a decent job at fitting the data and therefore we can be satisfied with it.

A word of caution

Polynomials are powerful tools but might backfire. In this case we knew that the original signal was generated using a third degree polynomial, however when analyzing real data, we usually know little about it and therefore we need to be cautious because the use of high order polynomials ($n > 4$) may lead to over-fitting. Over-fitting happens when your model is picking up the noise instead of the signal. Even though your model is getting better and better at fitting the existing data, this can be bad when you are trying to predict new data and lead to misleading results.