Fitting Curves to Data

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Contents

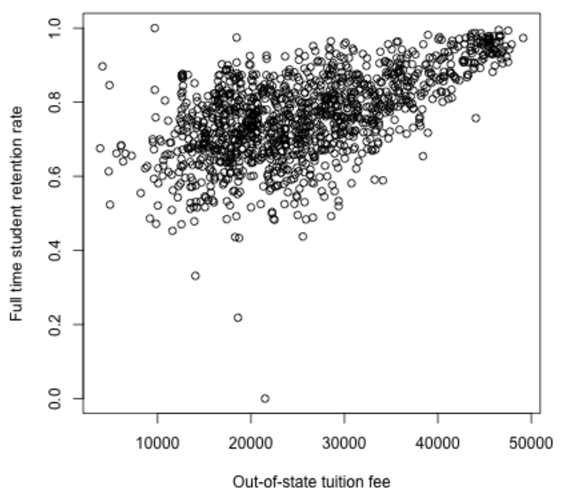
Comparing groups evaluates how a **continuous variable** (often called the response or independent variable) is related to a **categorical variable**. In our flight example, the continuous variable is the flight delay and the categorical variable is which airline carrier was responsible for the flight.

Now let us turn to relating two continuous variables. We will review the method that you've learned already – simple linear regression – and briefly discuss inference in this scenario. Then we will turn to expanding these ideas for more flexible curves than just a line.

1 Linear regression with one predictor

Let's consider the following data collected by the Department of Education regarding undergraduate institutions in the 2013-14 academic year (`https://catalog.data.gov/dataset/college-scorecard`). The department of education collects a great deal of data regarding the individual colleges/universities (including for-profit schools). Let's consider two variables, the tuition costs and the retention rate of students (percent that return after first year). We will exclude the for-profit institutes (there aren't many in this particular data set), and focus on out-of-state tuition to make the values more comparable between private and public institutions.

```
dataDir <- "../../finalDataSets"
scorecard <- read.csv(file.path(dataDir, "college.csv"),
    stringsAsFactors = FALSE)
scorecard <- scorecard[-which(scorecard$CONTROL ==
    3), ]
xlab = "Out-of-state tuition fee"
ylab = "Full time student retention rate"
plot(scorecard[, c("TUITIONFEE_OUT", "RET_FT4")], xlab = xlab,
    ylab = ylab)
```



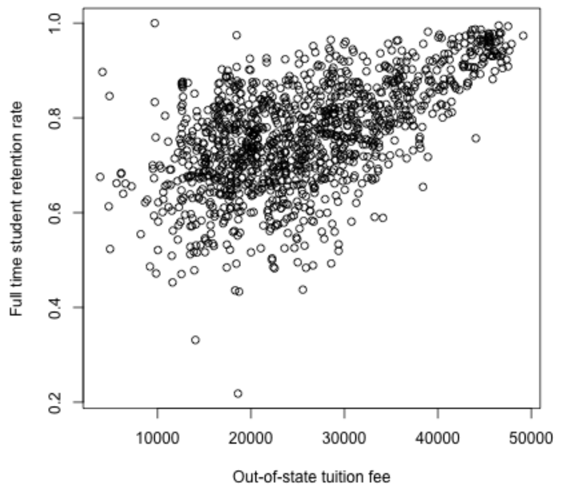
What do you observe in these relationships?

It's not clear what's going on with this observation with 0% return rate, but a 0% return rate is an unlikely value for an accreditated institution and is highly likely to be an error. So for now we'll drop that value. This is not something we want to do lightly, and points to the importance of having some understanding of the data – knowing that *a priori* 0% is a suspect number, for example. But just looking at the plot, it's not particularly clear that 0% is any more "outlying" than other points; we're basing this on our knowledge that 0% returning after the first year seems quite surprising. If we look at the college (Pennsylvania College of Health Sciences), a google search shows that it changed it's name in 2013 which is a likely cause.

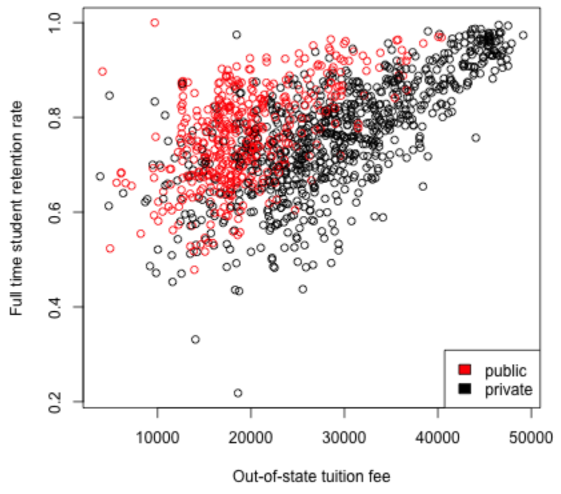
```
scorecard[scorecard[, "RET_FT4"] == 0, ]
```

```
##         X                                 INSTNM STABBR ADM_RATE_ALL
## 1238 5930 Pennsylvania College of Health Sciences     PA          398
##      SATMTMID SATVRMID SAT_AVG_ALL AVGFACSAL TUITFTE TUITIONFEE_IN
## 1238      488      468         955      5728   13823         21502
##      TUITIONFEE_OUT CONTROL UGDS UGDS_WHITE UGDS_BLACK UGDS_HISP
## 1238          21502       2 1394     0.8364     0.0445    0.0509
##      UGDS_ASIAN UGDS_AIAN UGDS_NHPI UGDS_2MOR UGDS_NRA UGDS_UNKN
## 1238     0.0294     7e-04    0.0029    0.0014        0    0.0337
##       INC_PCT_LO  INC_PCT_M1  INC_PCT_M2  INC_PCT_H1  INC_PCT_H2 RET_FT4
## 1238 0.367788462 0.146634615 0.227163462 0.175480769 0.082932692       0
##      PCTFLOAN C150_4 mn_earn_wne_p10 md_earn_wne_p10 PFTFAC
## 1238   0.6735 0.6338           53500           53100 0.7564
```

```
scorecard <- scorecard[-which(scorecard[, "RET_FT4"] ==
    0), ]
plot(scorecard[, c("TUITIONFEE_OUT", "RET_FT4")], xlab = xlab,
    ylab = ylab)
```



What do I see if I color the universities by whether they are private or not?



This highlights why it is very important to use more than one variable in trying to understand patterns or predict, which we will spend much more time on later in the course. But for now we are going to focus on one variable analysis, so lets make this a more valid exercise by just considering private schools.

```r
private <- subset(scorecard, CONTROL == 2)
public <- subset(scorecard, CONTROL == 1)
```

1.1 Estimating a Linear Model

These are convenient variables to consider the simplest relationship you can imagine for the two variables – a linear one:

$$y = \beta_0 + \beta_1 x$$

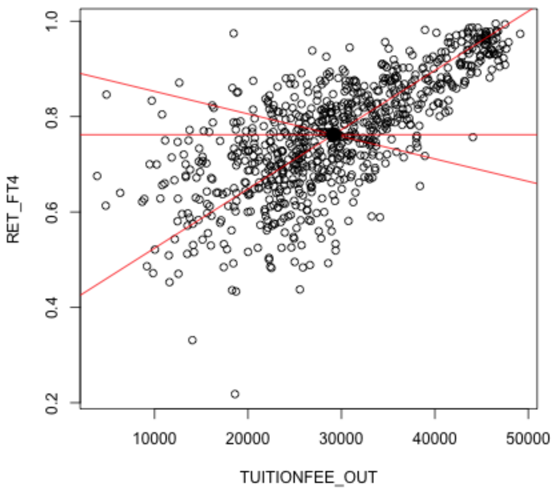
Of course, this assumes there is no noise, so instead, we often write

$$y = \beta_0 + \beta_1 x + e$$

where e represents some noise that gets added to the $\beta_0 + \beta_1 x$; e explains why the data do not exactly fall on a line.[1]

We do not know β_0 and β_1. They are parameters of the model. We want to estimate them from the data.

How to estimate the line There are many possible lines, of course, even if we force them to go through the middle of the data (e.g. the mean of x,y)



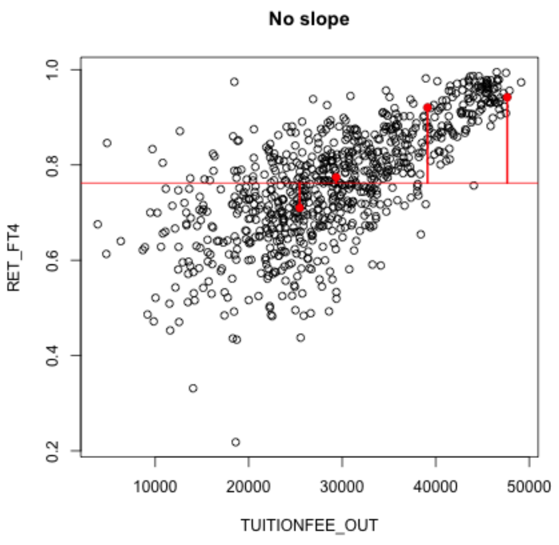
[1]It is useful to remember that *adding* noise is not the only option – this is a *choice* of a model.

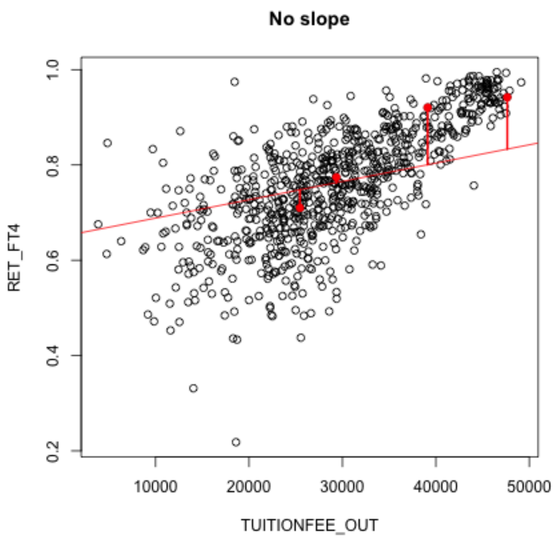
How do we decide which line is best? A reasonable choice is one that makes the smallest errors in predicting the response y. For each possible β_0, β_1 pair (i.e. each line), we can calculate the prediction from the line,

$$\hat{y}(\beta_0, \beta_1, x) = \beta_0 + \beta_1 x$$

and compare it to the actual observed y. Then we can say that the error in prediction for the point (x_i, y_i) is given by

$$y_i - \hat{y}(\beta_0, \beta_1, x_i)$$





Of course, for any particular point (x_i, y_i), we can choose a β_0 and β_1 so that $\beta_0 + \beta_1 x_i$ is *exactly* y_i. But that would only be true for one point; we want to find a *single* line that seems "good" for all the points.

We need a measure of the **fit** of the line to all the data. We do this by taking the average error across all the points. This gives us a measure of the total amount of error for a possible line.

1.2 Choise of error (loss function)

Using our error from above (the difference of y_i and $\hat{y}_i$), would give us the average error of

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)$$

But notice that there's a problem with this. Our errors are allowed to cancel out, meaning a very large positive error coupled with a very large negative error cancel each other and result in no measured error! That's not a promising way to pick a line – we want every error to count. So we want to have a strictly positive measure of error so that error's will accumulate.

The choice of how to quantify the error (or loss) is called the **loss function**, $\ell(y, \hat{y}(\beta_0, \beta_1))$. There are two common choices for this problem

- **Absolute loss**
$$\ell(y_i, \hat{y}_i) = |y_i - \hat{y}_i(\beta_0, \beta_1)|$$
- **Squared-error loss**
$$\ell(y_i, \hat{y}_i) = (y_i - \hat{y}_i(\beta_0, \beta_1))^2$$

Then our overall fit is given by

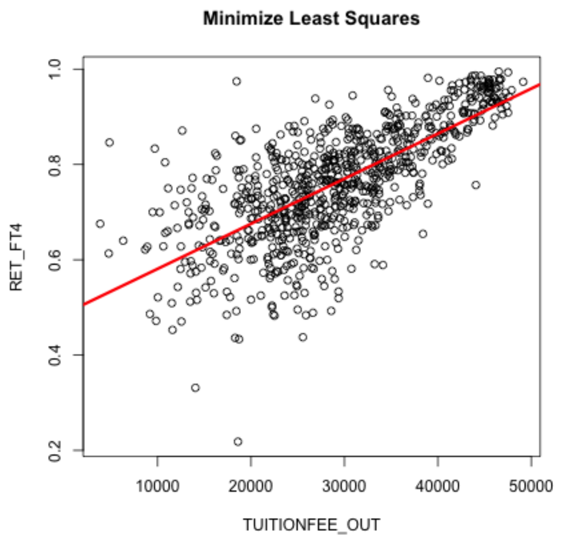
$$\frac{1}{n}\sum_{i=1}^{n} \ell(y_i, \hat{y}_i(\beta_0, \beta_1))$$

1.3 Squared-error loss

The most commonly used loss is squared-error loss, also known as **least squares regression**, where our measure of overall error for any particular β_0, β_1 is the average squared error,

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i(\beta_0, \beta_1))^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i)^2$$

We can find the β_0 and β_1 that minimize the least-squared error, using the function `lm` in R. We call these values we find $\hat{\beta}_0$ and $\hat{\beta}_1$. Below we draw the prediced line:



What do you notice about this line?

```
lm(RET_FT4 ~ TUITIONFEE_OUT, data = private)
```

```
##
## Call:
## lm(formula = RET_FT4 ~ TUITIONFEE_OUT, data = private)
##
## Coefficients:
##    (Intercept)  TUITIONFEE_OUT
##      4.863e-01       9.458e-06
```

```
lmPrivate <- lm(RET_FT4 ~ TUITIONFEE_OUT, data = private)
names(lmPrivate)
```

```
##  [1] "coefficients"  "residuals"     "effects"       "rank"
##  [5] "fitted.values" "assign"        "qr"            "df.residual"
##  [9] "xlevels"       "call"          "terms"         "model"
```

```
lmPrivate$coefficients
```

```
##    (Intercept) TUITIONFEE_OUT
##   4.863443e-01   9.458235e-06
```

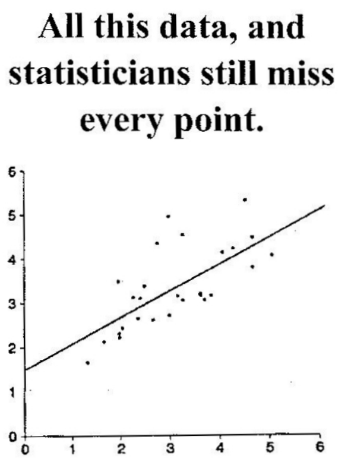
```r
coef(lmPrivate)
```

```
##    (Intercept) TUITIONFEE_OUT
##   4.863443e-01   9.458235e-06
```

How do you interpret the coefficients?

How much predicted increase in do you get for an increase of $10,000 in tuition?

Notice, as the below graphic jokes, the goal is not to exactly fit any particular point, and our line might not actually go through any particular point.[2]



[2]The above graphic comes from the 1999 winner of the annual statistics department contest for tshirt designs

The estimates of β_0 and β_1 If we want we can write down the equation for $\hat{\beta}_1$ and $\hat{\beta}_0$ (you don't need to memorize these equations)

$$\begin{aligned}\hat{\beta}_1 &= \frac{\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2}\\ \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1\bar{x}\end{aligned}$$

What do you notice about the denominator of $\hat{\beta}_1$?

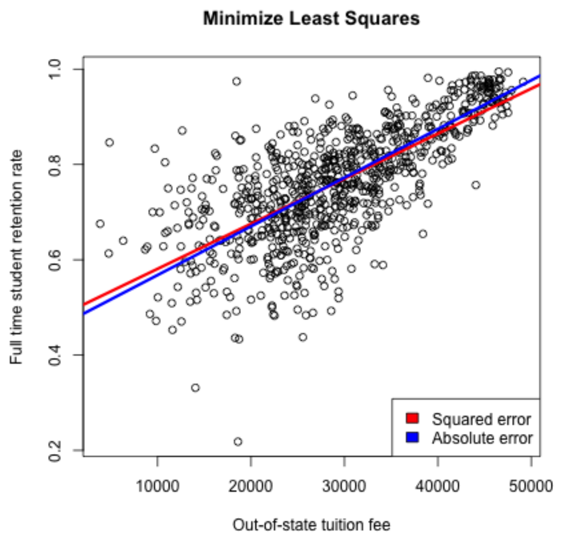
The numerator is also an average, only now it's an average over values that involve the relationship of x and y. Basically, the numerator is large if for the same observation i, both x_i and y_i are far away from their means, with large positive values if they are consistently in the same direction and large negative values if they are consistently in the opposite direction from each other.

1.4 Absolute Errors

Least squares is quite common, particularly because it quite easily mathematically to find the solution. However, it's equally compelling to use the absolute error loss, rather than squared error, which gives us a measure of overall error as:

$$\frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}(\beta_0, \beta_1)|$$

We can't write down the equation for the $\hat{\beta}_0$ and $\hat{\beta}_1$ that makes this error the smallest possible, but we can find them using the computer, which is done by the `rq` function in R.



While least squares is more common for historical reasons (we can write down the solution!), using absolute error is in many ways more compelling, just like the median can be better than the mean for summarizing the distribution of a population. With squared-error, large differences become even larger, increasing the influence of outlying points, because reducing the squared error for these outlying points will significantly reduce the overall average error.

We will continue with the traditional least squares, since we are not (right now) going to spend very long on regression before moving on to other techniques for dealing with two continuous variables.

2 Inference for linear regression

One question of particular interest is determining whether $\beta_1 = 0$. Why? (Consider this data on college tuition – what does $\beta_1 = 0$ imply)?

We can use the same strategy of inference for asking this question – hypothesis testing, p-values and confidence intervals.

As a hypothesis test, we have a null hypothesis of:

$$H_0 : \beta_1 = 0$$

We can also set up the hypothesis

$$H_0 : \beta_0 = 0$$

However, this is (almost) never interesting. Consider our data: what would it mean to have $\beta_0 = 0$?

Does this mean we can just set β_0 to be anything, and not worry about it?

2.1 Bootstrap Confidence intervals

Once we get estimates $\hat{\beta}_0$ and $\hat{\beta}_1$, how can we get bootstrap confidence intervals for the estimates?

```
bootstrapLM <- function(y, x, repetitions, confidence.level = 0.95) {
    stat.obs <- coef(lm(y ~ x))
    bootFun <- function() {
        sampled <- sample(1:length(y), size = length(y),
            replace = TRUE)
        coef(lm(y[sampled] ~ x[sampled]))
    }
    stat.boot <- replicate(repetitions, bootFun())
    nm <- deparse(substitute(x))
    row.names(stat.boot)[2] <- nm
    level <- 1 - confidence.level
    confidence.interval <- apply(stat.boot, 1, quantile,
        probs = c(level/2, 1 - level/2))
    return(list(confidence.interval = cbind(lower = confidence.interval[1,
        ], estimate = stat.obs, upper = confidence.interval[2,
        ]), bootStats = stat.boot))
}
```

```
privateBoot <- with(private, bootstrapLM(y = RET_FT4,
    x = TUITIONFEE_OUT, repetitions = 10000))
privateBoot$conf
```

```
##                        lower     estimate        upper
## (Intercept)    4.628622e-01 4.863443e-01 5.094172e-01
## TUITIONFEE_OUT 8.766951e-06 9.458235e-06 1.014341e-05
```

```
privateBoot[["confidence.interval"]]
```

```
##                        lower     estimate        upper
## (Intercept)    4.628622e-01 4.863443e-01 5.094172e-01
## TUITIONFEE_OUT 8.766951e-06 9.458235e-06 1.014341e-05
```

```
privateBoot[["conf"]]
```

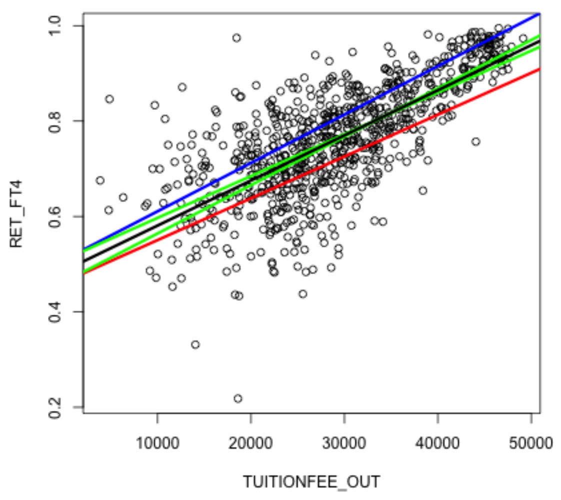
```
## NULL
```

```
privateBoot$conf[2, ] * 10000
```

```
##      lower   estimate      upper
## 0.08766951 0.09458235 0.10143414
```

How do we interpret these confidence intervals? What do they tell us about the problem?

```
plot(private[, c("TUITIONFEE_OUT", "RET_FT4")], col = "black")
abline(a = privateBoot$conf[1, 1], b = privateBoot$conf[2,
    1], col = "red", lwd = 3)
abline(a = privateBoot$conf[1, 3], b = privateBoot$conf[2,
    3], col = "blue", lwd = 3)
abline(a = privateBoot$conf[1, 1], b = privateBoot$conf[2,
    3], col = "green", lwd = 3)
abline(a = privateBoot$conf[1, 3], b = privateBoot$conf[2,
    1], col = "green", lwd = 3)
abline(lmPrivate, lwd = 3)
```



In principle, anything in this range is covered by the confidence intervals. However, that is not quite true. Our confidence in where the line is actually is narrower than what is shown, because some of the combinations of values of the two confidence intervals don't actually ever get seen together – these two statistics aren't independent from each other. Separate confidence intervals for the two values don't give you that information.[3]

2.2 Parametric Models

If we look at the summary of the `lm` function that does linear regression in R, we see a lot of information beyond just the estimates of the coefficients:

```
summary(lmPrivate)
```

```
##
## Call:
## lm(formula = RET_FT4 ~ TUITIONFEE_OUT, data = private)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.44411 -0.04531  0.00525  0.05413  0.31388
##
## Coefficients:
```

[3]You can actually have joint confidence regions that demonstrate the dependency between these values, but that is beyond this class.

```
##                  Estimate Std. Error t value Pr(>|t|)
## (Intercept)    4.863e-01  1.020e-02   47.66   <2e-16 ***
## TUITIONFEE_OUT 9.458e-06  3.339e-07   28.32   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.08538 on 783 degrees of freedom
## Multiple R-squared:  0.5061,Adjusted R-squared:  0.5055
## F-statistic: 802.3 on 1 and 783 DF,  p-value: < 2.2e-16
```

We see that it automatically spits out a table of estimated values and p-values along with a lot of other stuff. This is exceedingly common – all statistical software programs do this – so let's cover the meaning of the most important components.

Null Hypotheses Why are there 2 p-values? What are the null hypotheses that these p-values correspond to?

Parametric Model for the data: `lm` uses a standard parametric model to get the distributions of our statistics $\hat{\beta}_0$ and $\hat{\beta}_1$.

Recall our linear model:

$$y = \beta_0 + \beta_1 x + e.$$

The standard parametric model for inference assumes a distribution for the errors e. Specifically, we assume

- $e \sim N(0, \sigma^2)$, i..e normal with the *same* (unknown) variance σ^2.
- The unknown errors $e_1, \ldots, e_n$ are all independent from each other

Notice, that means for a given x_i, each y_i is normally distributed, since it is just a normal (e_i) with a (unknown) constant added to it ($\beta_0 + \beta_1 x_i$). So

$$y_i | x_i \sim N(\beta_0 + \beta_1 x_i, \sigma^2)$$

However, even though the errors e_i are assumed *i.i.d* the y_i are not i.i.d, why?

This assumption regarding the distribution of the errors allows us to know the distribution of the $\hat{\beta}_1$. We won't show this, but since each y_i is normally distributed, the $\hat{\beta}_1$ is as well.[4]

$$\hat{\beta}_1 \sim N(\beta_1, \nu_1^2)$$

where

$$\nu_1^2 = var(\hat{\beta}_1) = \frac{\sigma^2}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

In what follows, just try to follow the logic, you don't need to memorize these equations or understand where they come from.

Notice the similarities in the broad outline of the parametric t-test for two-groups. We have an statistic, $\hat{\beta}_1$, and the assumptions of the parametric model gives us the distribution of $\hat{\beta}_1$.

Estimating σ^2 Of course, we have the same problem as the t-test – we don't know σ^2! But we can estimate σ^2 too and get an estimate of the variance (we'll talk more about how we estimate $\hat{\sigma}$ when we return to linear regression with multiple variables)

$$\hat{\nu}_1^2 = v\hat{a}r(\hat{\beta}_1 = \frac{\hat{\sigma}^2}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

Hypothesis Testing Using this, we can use the same idea as the t-test for two-groups, and create a similar test statistic for $\hat{\beta}_1$ that standardizes $\hat{\beta}_1$[5]

$$T_1 = \frac{\hat{\beta}_1}{\sqrt{v\hat{a}r(\hat{\beta}_1)}}$$

Just like the t-test, T_1 should be normally distributed[6] This is exactly what `lm` gives us:

```
summary(lm(RET_FT4 ~ TUITIONFEE_OUT, data = private))
```

```
##
## Call:
## lm(formula = RET_FT4 ~ TUITIONFEE_OUT, data = private)
##
```

[4]If you look at the equation of $\hat{\beta}_1$, then we can see that it is a linear combination of the y_i, and linear combinations of normal R.V. are normal, even if the R.V. are not independent.

[5]In fact, we can also do this for $\hat{\beta}_0$, with exactly the same logic, though β_0 is not interesting.

[6]with the same caveat, that when you estimate the variance, you affect the distribution of T_1, which matters in small sample sizes.

```
## Residuals:
##      Min       1Q   Median       3Q      Max 
## -0.44411 -0.04531  0.00525  0.05413  0.31388 
## 
## Coefficients:
##                 Estimate Std. Error t value Pr(>|t|)    
## (Intercept)    4.863e-01  1.020e-02   47.66   <2e-16 ***
## TUITIONFEE_OUT 9.458e-06  3.339e-07   28.32   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## 
## Residual standard error: 0.08538 on 783 degrees of freedom
## Multiple R-squared:  0.5061,Adjusted R-squared:  0.5055 
## F-statistic: 802.3 on 1 and 783 DF,  p-value: < 2.2e-16
```

Confidence intervals We can also create parametric confidence intervals for $\hat{\beta}_1$ in the same way we did for two groups:

$$\hat{\beta}_1 \pm 1.96\hat{\nu}_1$$

```
confint(lmPrivate)
```

```
##                       2.5 %       97.5 %
## (Intercept)    4.663136e-01 5.063750e-01
## TUITIONFEE_OUT 8.802757e-06 1.011371e-05
```

2.2.1 Estimating σ^2

How do we estimate σ^2? Recall that σ^2 is the variance of the error distribution. We don't know the true errors e_i, but if we did, we know they are i.i.d and so a good estimate of σ^2 *would be* the sample variance of the true errors:

$$\frac{1}{n-1}\sum(e_i - \bar{e})^2$$

However, these true errors are unknown. If we knew the true β_0 and β_1 we could calculate the true e_i, how?

But these coefficeints are also unknown. Yet, this does give us the idea that we do have some idea of the errors since we have estimates of β_0 and β_1. Namely, we can calculate the error of our data from the *estimated* line,

$$r_i = y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i)$$

The r_i are called the **residuals**. They are often called the errors, but they are not the actual (true) error, however. They are the error from the *estimated* line.

Using the residuals, we can take the sample variance of the residuals as a good first estimate of σ^2,

$$\frac{1}{n-1}\sum(r_i - \bar{r})^2$$

Mean of residuals, $\bar{r}$ In fact, it is an algebraic fact that $\bar{r} = 0$. But, this is NOT a sign the line is a good fit. It is just always true, even when the line is a lousy fit to the data.

Better estimate of σ Moreover, for regression, a better estimate is to divide by $n-2$ rather than $n-1$. Doing so makes our estimate **unbiased**, meaning that the average value of $\hat{\sigma}^2$ over many repeated samples will be σ. This is the same reason we divide by $n-1$ in estimating the sample variance rather than $1/n$ for the estimate of the variance of a single population.

These two facts gives us our final estimate:

$$\hat{\sigma}^2 = \frac{1}{n-2}\sum_i r_i^2.$$

The residuals r_i are not always great estimates of e_i (for example, they aren't independent, they don't have the same variance, etc). But, despite that, it turns out that $\hat{\sigma}^2$ is a very good estimate of σ^2, even if the errors aren't normal.

2.3 Assumptions

Like the t-test, the bootstrap gives a more robust method than the parametric linear model for creating confidence intervals.

The parametric linear model makes the following assumptions:

- Errors e_i are independent

- Errors e_i are i.i.d, meaning they have the same variance
- Errors are normally distributed

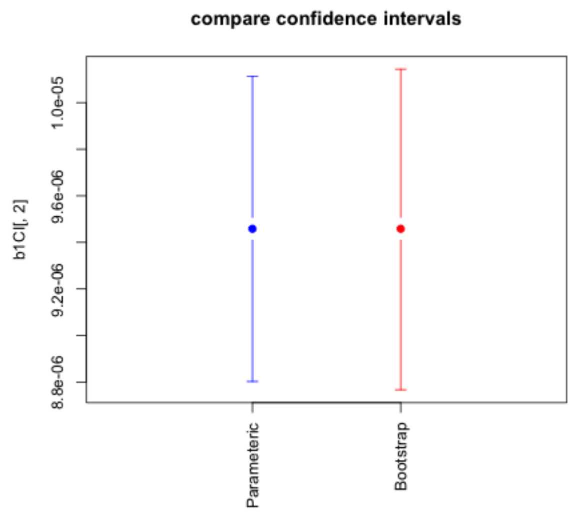
The bootstrap makes the same kind of assumptions as with the two group comparisons:

- The i.i.d resampling of the bootstrapped data mirrors how the actual data was generated (i.e. actual data was i.i.d)
- The sample size is large enough that the sample distribution is close to the real distribution.
- The test statistic is well behaved (e.g. unbiased) – and this is true for regression

Notice, that both methods assume the data points are *independent*. This is the most critical assumption for both methods. Both implicitly assume that all of the observations have the same variance (i.i.d). The parametric method makes the further assumption of normality of the errors (like the t-test).

In practice, we do not see much difference in these two methods for our data:

```
##             lower     estimate        upper
## [1,] 8.802757e-06 9.458235e-06 1.011371e-05
## [2,] 8.766951e-06 9.458235e-06 1.014341e-05
```



2.4 Prediction Intervals

In addition to evaluating the coefficients, we can also look at the prediction we would make. This is better way than the plots we did from the confidence intervals to get an idea of what our predictions at a particular value would actually be.

Prediction How does our model a value, say for tuition of $20,000?

```
coef(lmPrivate)[1] + coef(lmPrivate)[2] * 20000
```

```
## (Intercept)
##    0.675509
```

```
predict(lmPrivate, newdata = data.frame(TUITIONFEE_OUT = 20000))
```

```
##        1
## 0.675509
```

These predictions are themselves statistics based on the data, and the uncertainty/variability in the coefficients carries over to the predictions. So we can also give confidence intervals for our prediction. There are two types of confidence intervals.

- Confidence intervals about the predicted average response – i.e. prediction of what is the average completion rate for all schools with tuition $20,000.
- Confidence intervals about a particular individual, i.e. prediction of a particular school that has tuition $20,000. These are actually not called confidence intervals, but **prediction intervals**.

Clearly, we predict the same estimate for both of these settings, but our estimate of the *precision* of these estimates varies. Which of these settings do you think would have wider CI?

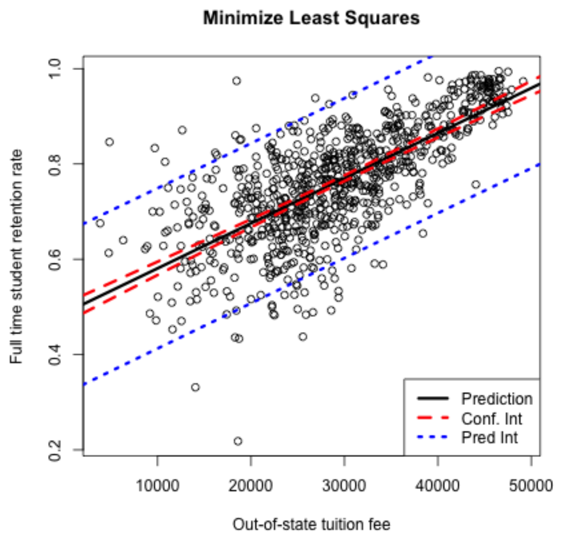
```r
predict(lmPrivate, newdata = data.frame(TUITIONFEE_OUT = 20000),
    interval = "confidence")
```

```
##         fit       lwr       upr
## 1 0.675509 0.6670314 0.6839866
```

```r
predict(lmPrivate, newdata = data.frame(TUITIONFEE_OUT = 20000),
    interval = "prediction")
```

```
##         fit       lwr      upr
## 1 0.675509 0.5076899 0.843328
```

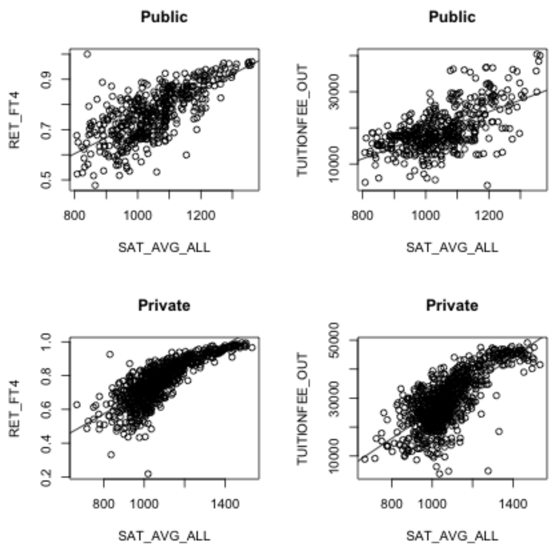
We can compare these two intervals by calculating them for a large range of x_i values and plotting them:



What do you notice about the difference in the confidence lines? How does it compare to the observed data?

3 Least Squares for Polynomial models & beyond

Least squares will spit out estimates of the coefficients and p-values to any data – the question is whether this is a good idea. For example, consider the variable `SAT_AVG_ALL` that gives the average SAT score for the school. Looking at the public institutions, what do you see as it's relationship to the other two variables?



We might imagine that other functions would be a better fit to the data for the private schools. What might be some reasonable choices of functions?

We can fit other functions in the same way. Take a quadratic function, for example. What does that look like for a model?

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + e$$

We can, again, find the best choices of those co-efficients by getting the predicted value for a set of coefficients:

$$\hat{y}_i(\beta_0, \beta_1, \beta_2) = \beta_0 + \beta_1 x_i + \beta_2 x_i^2,$$

and find the error

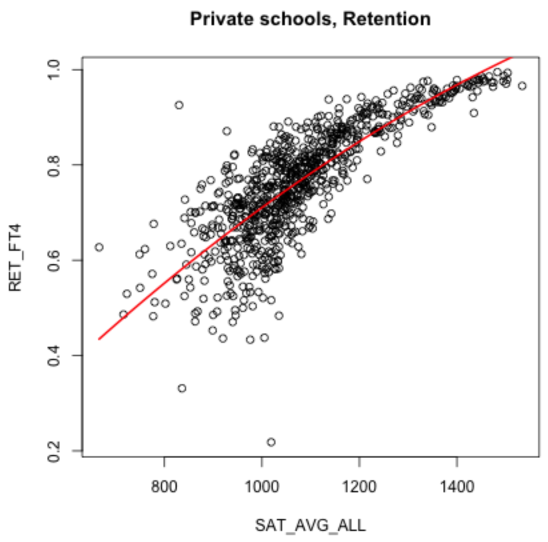
$$\ell(y_i, \hat{y}_i(\beta_0, \beta_1, \beta_2))$$

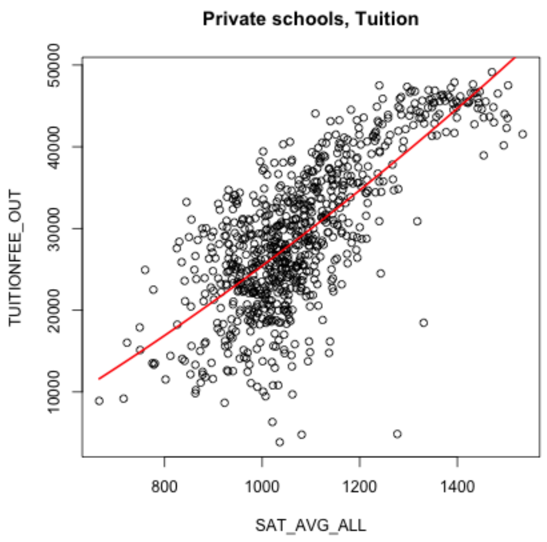
and trying to find the choices that minimizes the average loss over all the observations.

If we do least squares for this quadratic model, we are trying to find the coefficients $\beta_0, \beta_1, \beta_2$ that minimize,

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i - \beta_2 x_i^2)^2$$

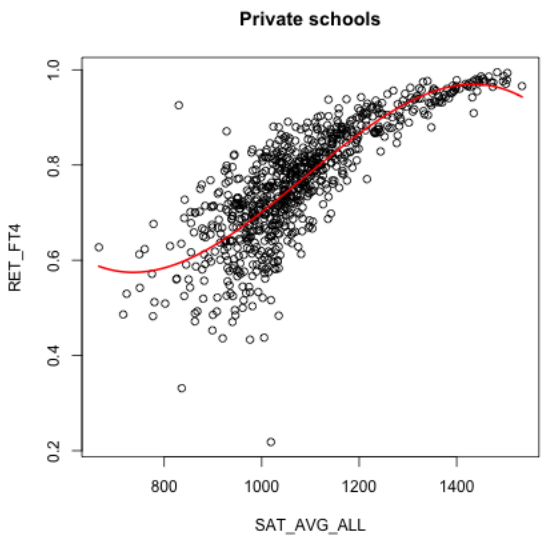
Here are the results:

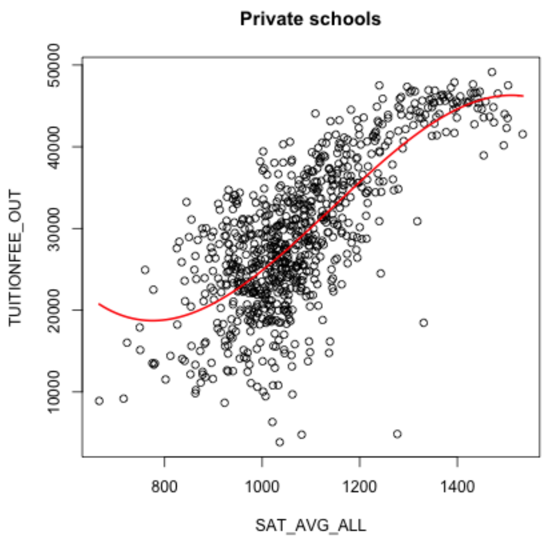




It's a little better, but not much. We could try other functions. A cubic function, for example, is exactly the same idea.

$$\hat{y}_i(\beta_0, \beta_1, \beta_2) = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3.$$





What do you think about the cubic fit?

4 Local fitting

Defining a particular function to match the entire scope of the data might be difficult. Instead we might want something that is more flexible. We'd really like to say

$$y = f(x) + e$$

and just estimate f, without any particular restriction on f.

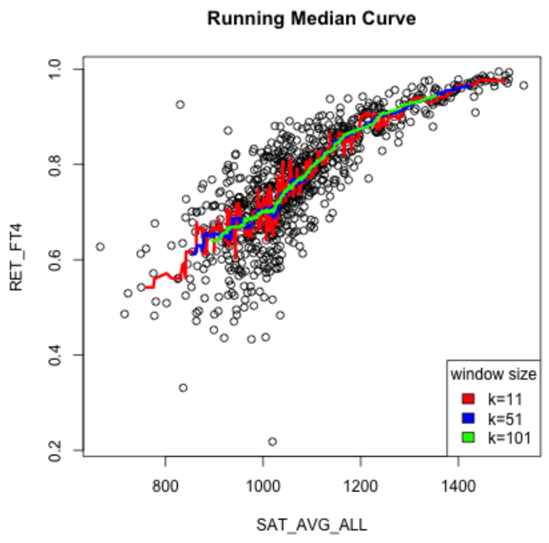
Like with density estimation, we are going to slowly build up to understanding the most commonly used method (LOESS) by starting with simpler ideas first. Brainstorm with a partner: what ideas can you imagine for how you might get a descriptive curve/line/etc to describe this data?

4.1 Running Mean or Median

One simple idea is to take a running mean or median over the data. In otherwords, take a window of points, and as you slide this window across the x-axis, take the mean.

$$\hat{f}(x) = \frac{1}{\text{\# in window}} \sum_{i:x_i \in [x-\frac{w}{2}, x+\frac{w}{2})} y_i$$

There are a lot of varieties on this same idea. For example, you could make the window not fixed width w, but a fixed number of points, etc. While it's conceptually easy to code from scratch, there are a lot of nitpicky details, so we'll use a built in implementation that does a fixed number of points.



What do you notice when I change the number of points in each window? Which seems more reasonable here?

Comparison to density estimation If this feels familiar, it should! This is very similar to what we did in density estimation. However, in estimating the density $p(x)$, we were taking data x_i that were in windows around x, and calculating the density estimate $\hat{p}(x)$ using basically just the *number* of points in the window

$$\hat{p}(x) = \frac{1}{nw\{\#\ x_i \text{ in window}\}} = \sum_{i:x_i \in [x-\frac{w}{2}, x+\frac{w}{2})} \frac{1}{nw}$$

With function estimation, we are finding the x_i that are near x and then taking their corresponding y_i to calculate $\hat{f}(x)$. So for function estimation, the x_i are used to determining which points (x_i, y_i) to use, but the y_i are used to calculate the value.

$$\begin{aligned}\hat{f}(x) &= \frac{\text{sum of } y_i \text{ in window}}{\#\ x_i \text{ in window}} \\ &= \frac{\sum_{i:x_i \in [x-\frac{w}{2}, x+\frac{w}{2})} y_i}{\sum_{i:x_i \in [x-\frac{w}{2}, x+\frac{w}{2})} 1}\end{aligned}$$

4.2 Kernel weighting

One disadvantage to a running median is that it can create a curve that is rather jerky as you add in one point/take away a point. Alternatively, if you have a wide window, then your curve at any point x will average the points that can be quite far away, and treat them equally as points that are nearby.

We've already seen a similar concept when we talked about kernel density estimation, instead of histograms. There we saw that we could describe our windows as *weighting* of our points x_i based on their distance from x. We can do the same idea for our running mean:

$$\begin{aligned}\hat{f}(x) &= \frac{\sum_{i:x_i \in [x-\frac{w}{2}, x+\frac{w}{2})} y_i}{\sum_{i:x_i \in [x-\frac{w}{2}, x+\frac{w}{2})} 1} \\ &= \frac{\sum_{i=1}^n y_i f(x, x_i)}{\sum_{i=1}^n f(x, x_i)}\end{aligned}$$

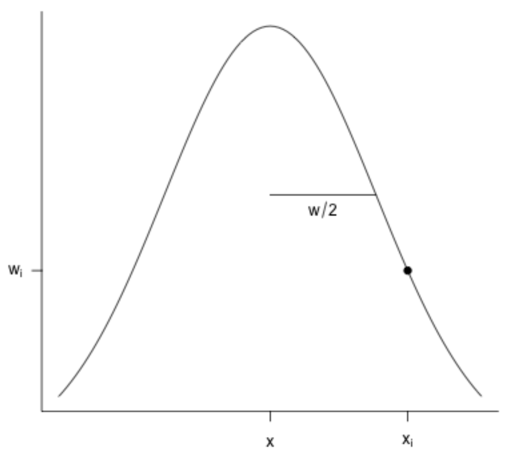
where again, $f(x, x_i)$ weights each point by $1/w$

$$f(x, x_i) = \begin{cases} \frac{1}{w} & x_i \in x_i \in [x - \frac{w}{2}, x + \frac{w}{2}) \\ 0 & otherwise \end{cases}$$

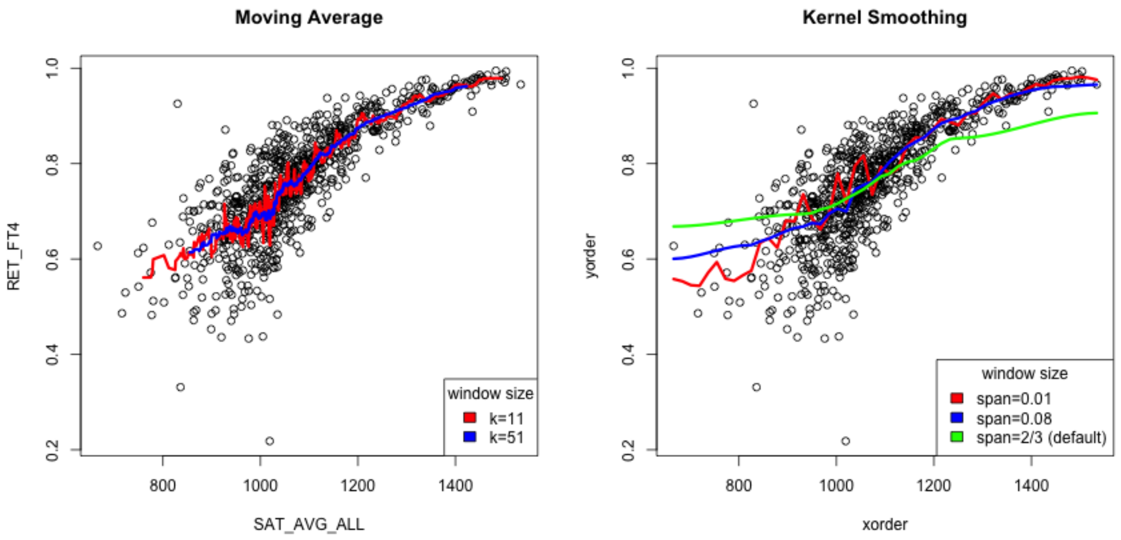
(notice the constant $1/w$ cancels out, but we leave it there to look like the kernel density estimation).

This is called the Nadaraya-Watson kernel-weighted average estimate or kernel smoothing regression.

Again, once we write it this way, it's clear we could again choose different weighting functions, like the gaussian kernel, similar to that of kernel density estimation. Just as in density estimation, you tend to get smoother results if our weights aren't abruptly changing from 0 once a point moves in or out of the window. So we will use the same idea, where we weight our point i based on how close x_i is to the x for which we are trying to estimate $f(x)$. And just like in density estimation, a gaussian kernel is the common choice for how to decide the weight:



Here's how the gaussian kernel smoothing weights compare to a rolling mean (i.e. based on fixed windows)



Window width The `span` argument tells you what percentage of points are used in predicting x (like bandwidth in density estimation)[7]. So there's still an idea of a window size; it's just that within the window, you are giving more emphasis to points near your x value.

Notice that one advantage is that you can define an estimate for any x in the

[7]There's a lot of details about span and what points are used, but we are not going to worry about them. What I've described here gets at the idea

range of your data – the estimated curve doesn't have to jump as you add new points. Instead it transitions smoothly.

What other comparisons might you make here?

Weighted Mean If we look at our estimate of $f(x)$, we can actually write it more simply as a **weighted mean** of our y_i

$$\hat{f}(x) = \frac{\sum_{i=1}^n y_i f(x, x_i)}{\sum_{i=1}^n f(x, x_i)} \\ = \sum_{i=1}^n w_i(x) y_i$$

where

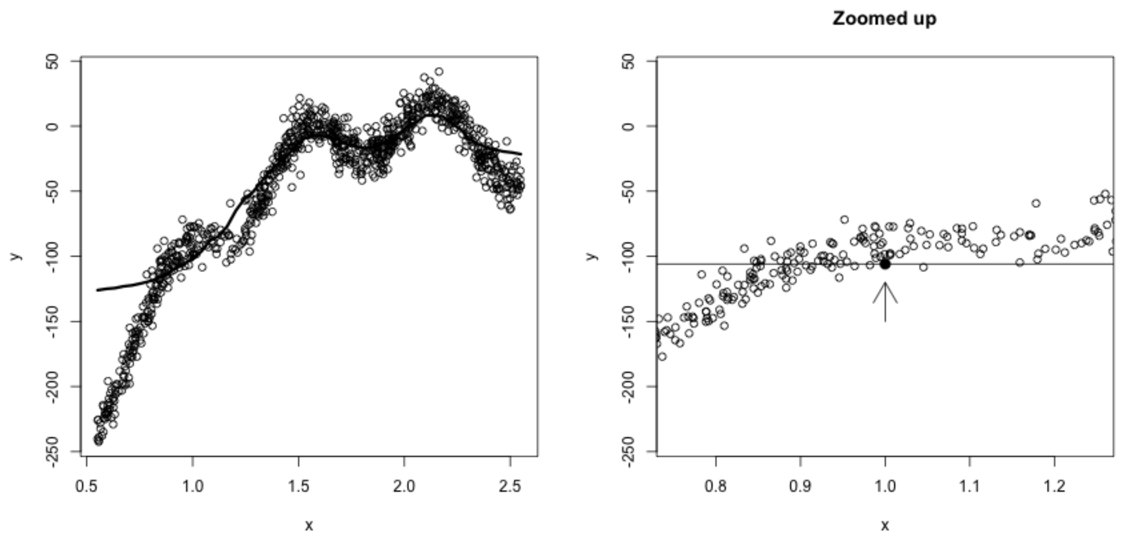
$$w_i(x) = \frac{f(x, x_i)}{\sum_{i=1}^n f(x, x_i)}$$

are weights that indicate how much each y_i should contribute to the mean (and notice that these weights sum to one). The standard mean of all the points is equivalent to choosing $w_i(x) = 1/n$, i.e. each point counts equally.

4.3 Loess: Local Regression Fitting

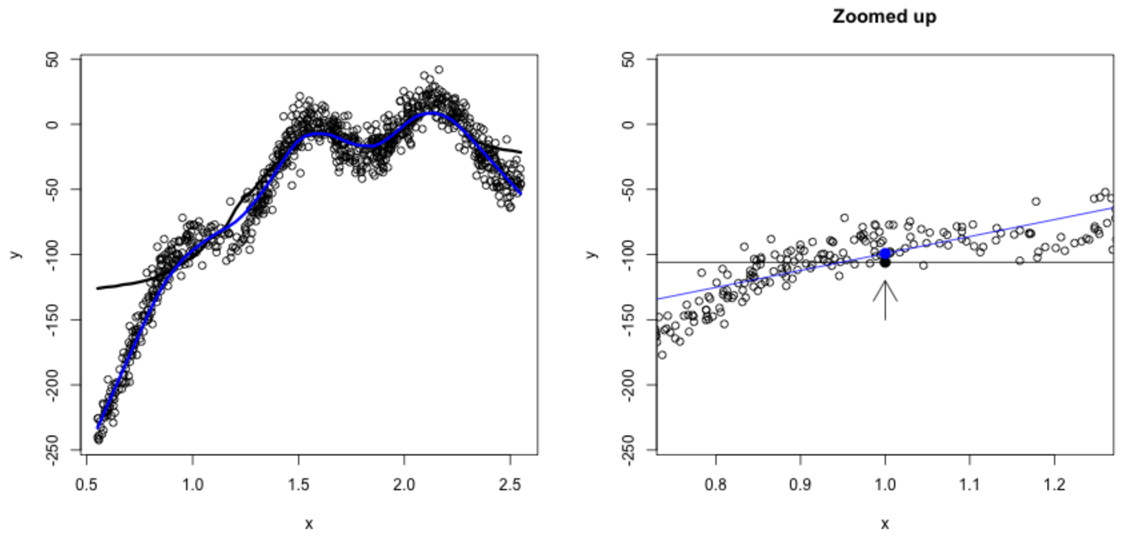
In the previous section, we use kernels to have a nice smooth way to decide how much impact the different y_i have in our estimate of $f(x)$. But we haven't changed the fact that we are essentially taking just a mean of the nearby y_i to estimate $f(x)$.

Let's go back to our simple windows (i.e. rectangular kernel). When we estimate $f(x)$, we are doing the following:

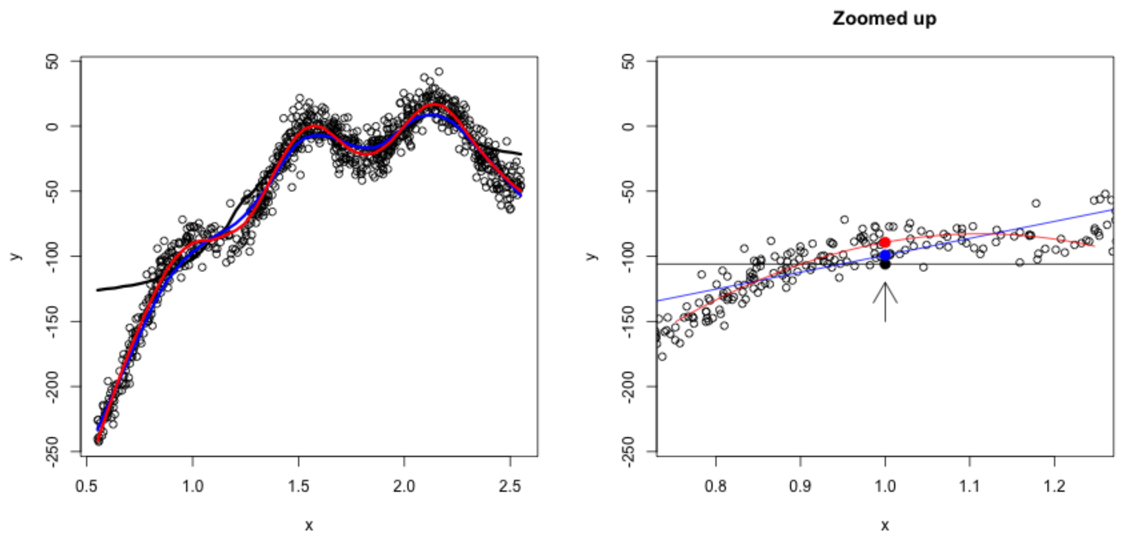


We see that for our prediction $\hat{f}(x)$ at $x = 1$, we are not actually getting into where the data is because of the in balance of how the x_i values are distributed. That's because the function is changing around $x = 1$; weighting far-away points would help some, we're basically trying to "fit" a constant line to what clearly is changing in this window.

We could do this for every x, as our window keeps moving, so we would never actually be fitting a polynomial across the entire function. So while we wouldn't think a line fit the overall data very well, locally around $x = 1$ it would be more reasonable to say it is roughly like a line:

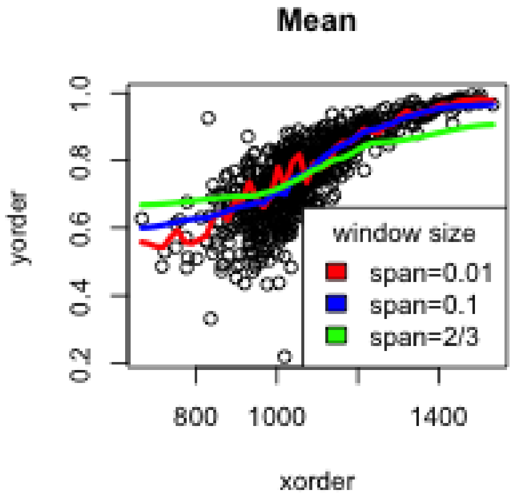


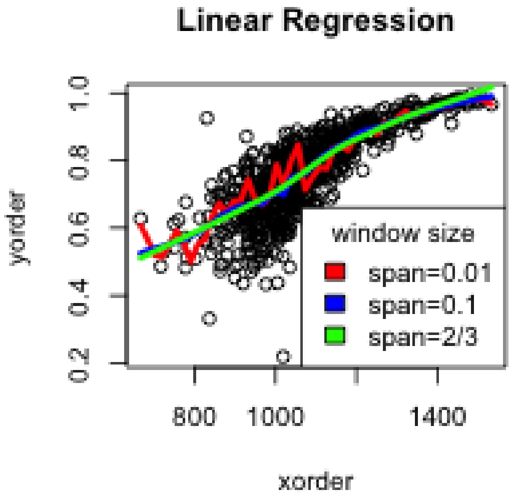
We could go even further and say a quadratic would be better:

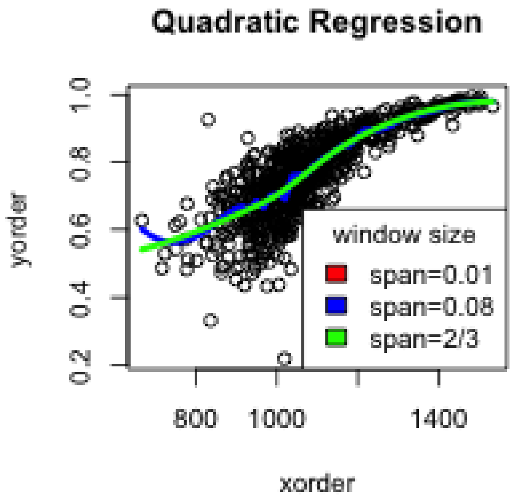


In short, we are saying, to estimate $f(x)$ *locally* some simple polynomials will work well, even though they don't work well globally.

So we now have the choice of the degree of the polynomial *and* the span/window size.





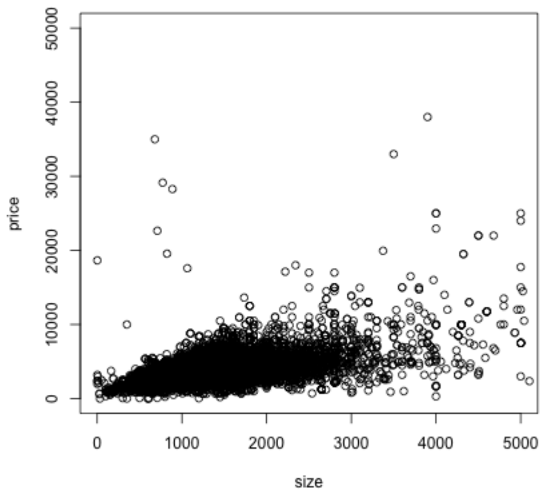


What conclusions would you draw about the difference between choosing the degree of the fit (mean/linear/quadratic)?

Generally degree is chosen to be 2, as it usually gives better fitting estimates, while the span parameter might be tweaked by the user.

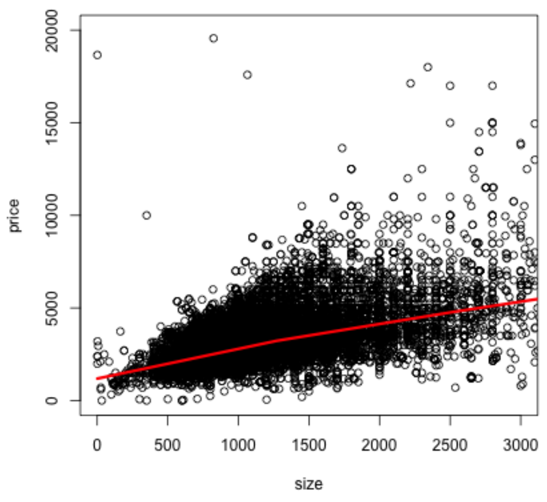
5 Big Data clouds

It can be particularly helpful to have a smooth scatter for visualization when you have a lot of data points. Consider the following data on craigs list rentals that you saw in lab. We would suspect that size would be highly predictive of price, and indeed if we plot price against size that's pretty clear.



But, because of the number of points, we can't really see much of what's going on. In fact our eye is drawn to outlying (and less representative) points, while the rest is just a black smear where the plots are on top of each other.

We can add a loess smooth curve to get an idea of where the bulk of the data lie. We'll zoom in a bit closer as well by changing the x and y limits of the axes.



What does this tell you about the data?

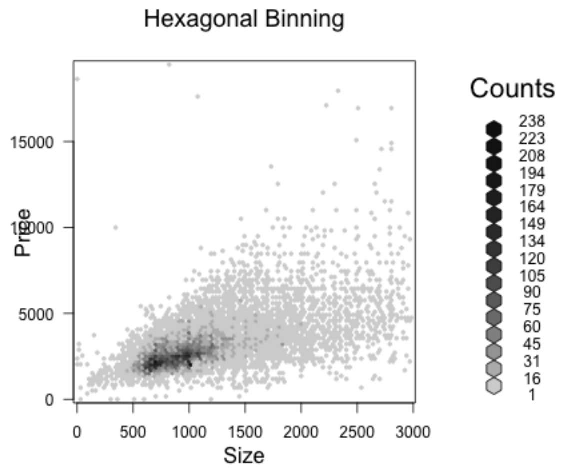
5.1 2D density smoothing plots

If we really want to get a better idea of what's going on under that smear of black, we can use 2D density smoothing plots. This is the same idea as density smoothing plots for probability densities, only for 2D. Imagine that instead of a histogram along the line, a 2D histogram. This would involve griding the 2D plane into rectangles (instead of intervals) and counting the number of points within each rectangle. The high of the bars (now in the 3rd dimension) would give a visualization of how many points there are in different places in the plot.

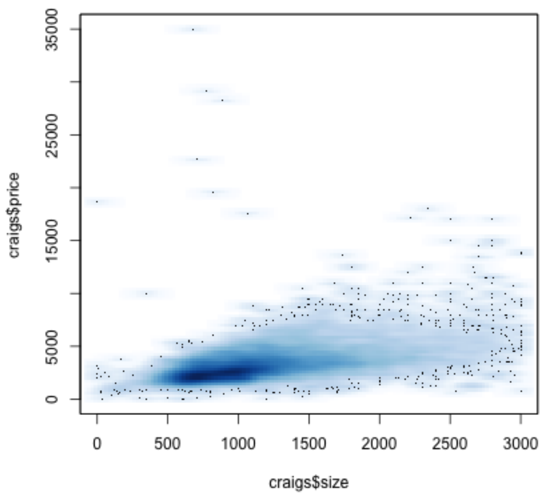
Then just like with histograms, we can smooth this, so that we get a smooth curve over the 2 dimensions.

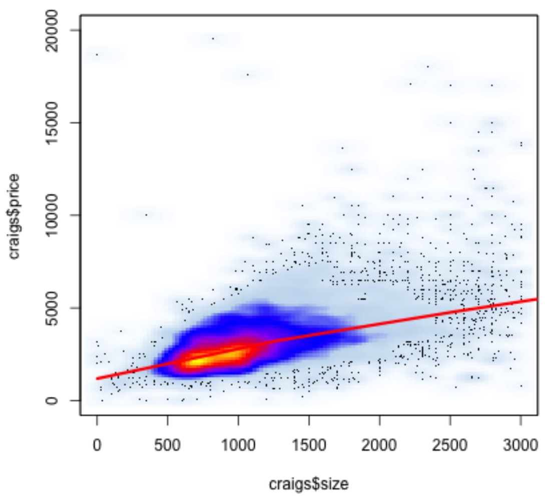
A 3D picture of this would be cool, but difficult to actually see information, axes, etc. So its common to instead smash this information into 2D, by representing the 3rd dimension (the density of the points) by a color scale instead.

Here is an example of such a visualization of a 2D histogram (the `hexbin` package)



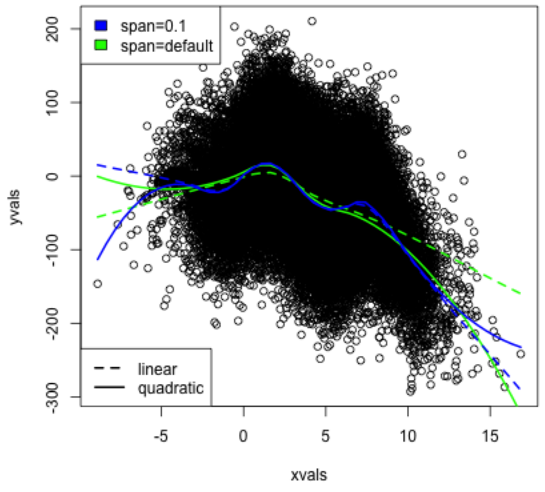
We can use a smoother version of this and get more gradual changes (and a less finicky function) using the `smoothScatter function`

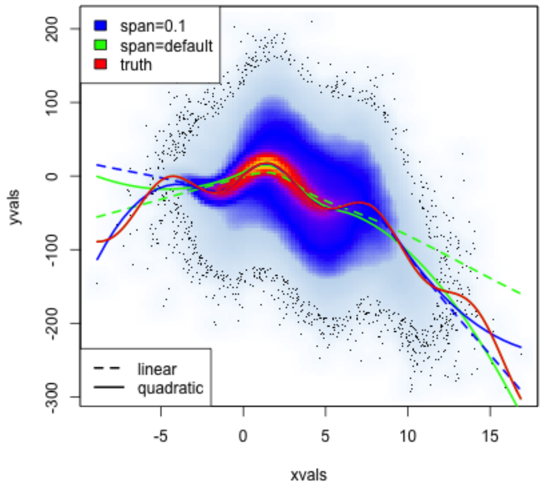


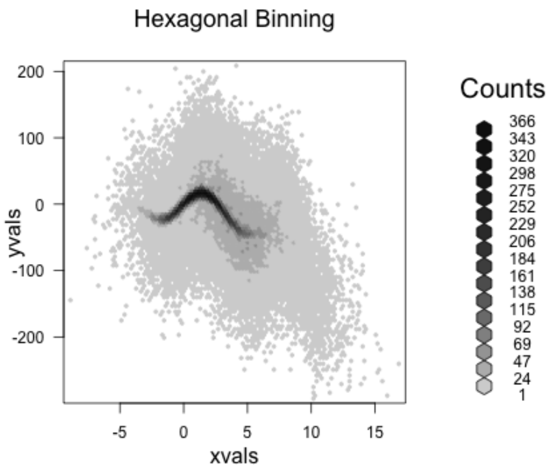


What do these colors tell you? How does this compare to the smooth line? What do you see about those points that grabbed our eye before (and which the loess line ignored)?

Simulated Example For this data, it turned out that the truth was pretty linear. But many times, the cloud of data can significantly impair our ability to see the data. We can simulate a more complicated function with many points.







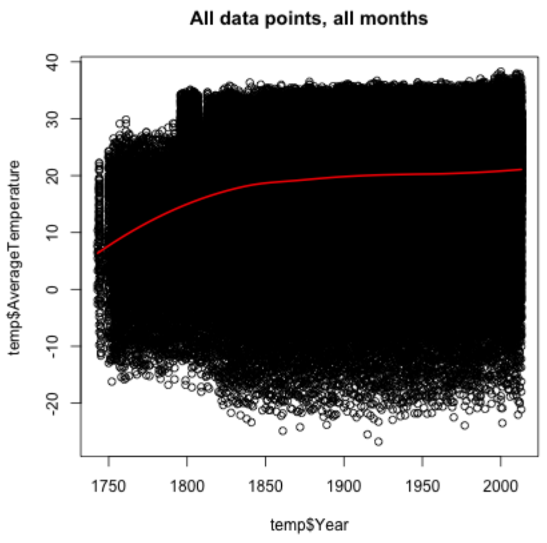
6 Time trends

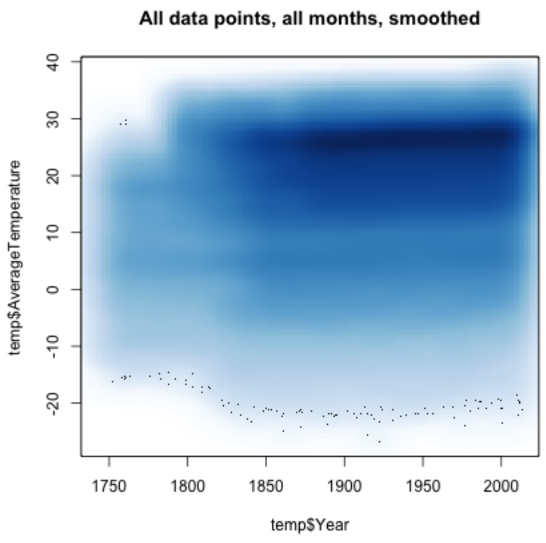
Let's look at another common example of fitting a trend – time data. In the following dataset, we have the average temperatures (in celecius) by city per month since 1743.

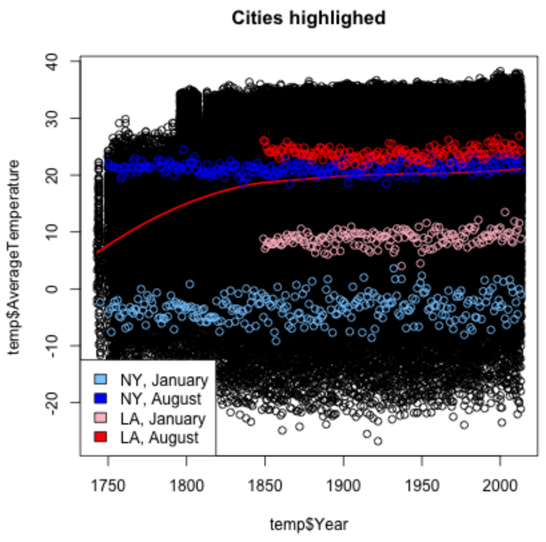
```
##           dt AverageTemperature AverageTemperatureUncertainty    City
## 1 1849-01-01             26.704                         1.435 Abidjan
## 2 1849-02-01             27.434                         1.362 Abidjan
## 3 1849-03-01             28.101                         1.612 Abidjan
## 4 1849-04-01             26.140                         1.387 Abidjan
## 5 1849-05-01             25.427                         1.200 Abidjan
## 6 1849-06-01             24.844                         1.402 Abidjan
##         Country Latitude Longitude
## 1 Côte D'Ivoire    5.63N     3.23W
## 2 Côte D'Ivoire    5.63N     3.23W
## 3 Côte D'Ivoire    5.63N     3.23W
## 4 Côte D'Ivoire    5.63N     3.23W
## 5 Côte D'Ivoire    5.63N     3.23W
## 6 Côte D'Ivoire    5.63N     3.23W
```

Given the scientific consensus that the planet is warming, it is interesting to look at this data, limited though it is, to see how different cities are affected.

Here, we plot the data with `smoothScatter`, as well as plotting just some specific cities

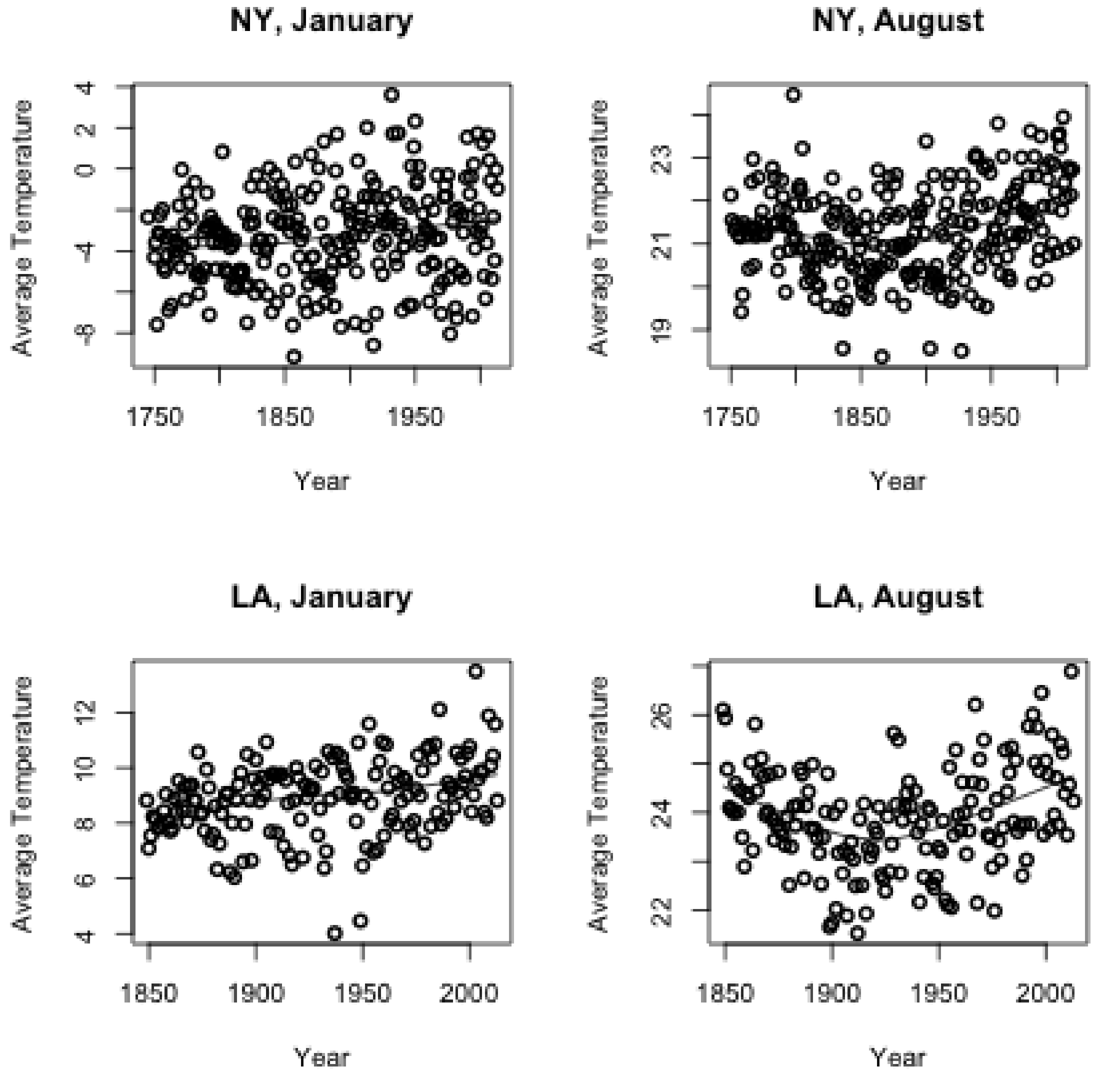






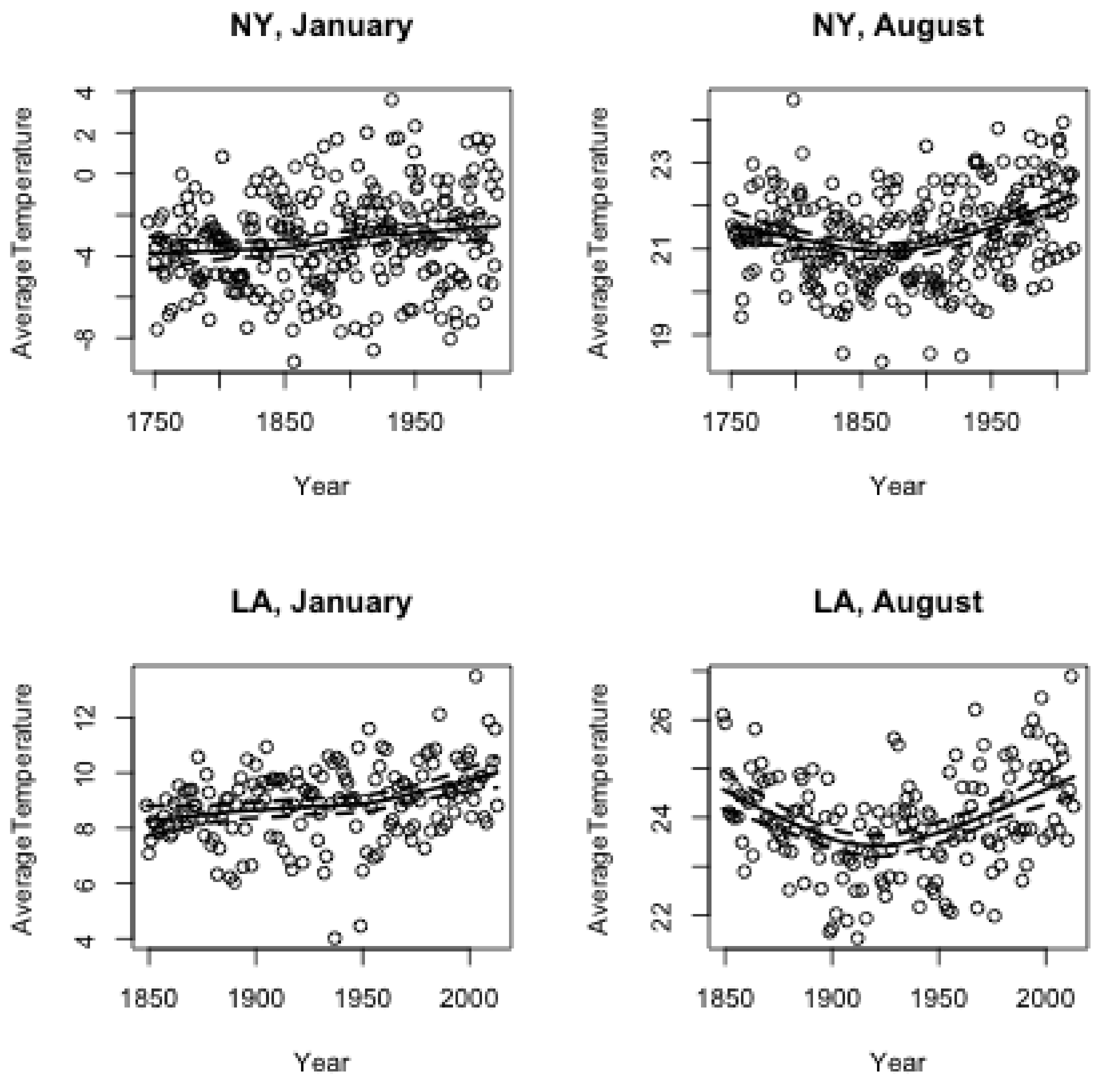
This is a very uninformative plot, despite our best efforts. Why?

We can consider for different cities or different months how average temperatures have changed. We use the function `scatter.smooth` that both plots the points and places a loess curve on top.



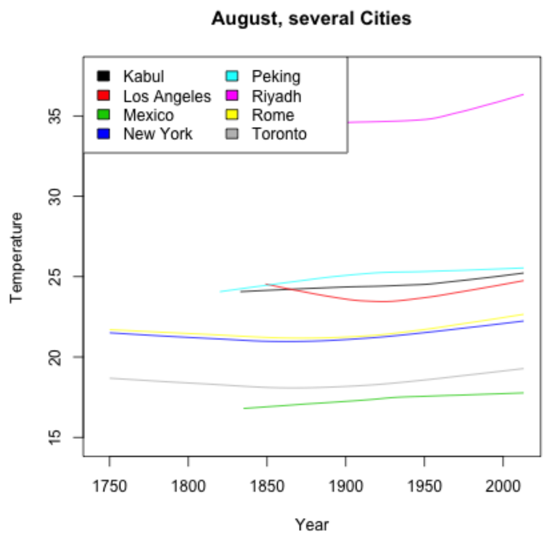
Loess Prediction Intervals We can even calculate (parametric) confidence intervals around these curves (based on a type of t-statistic for kernel smoothers), with a bit more lines of code. They are called prediction intervals, because they are confidence intervals for the prediction at each point.

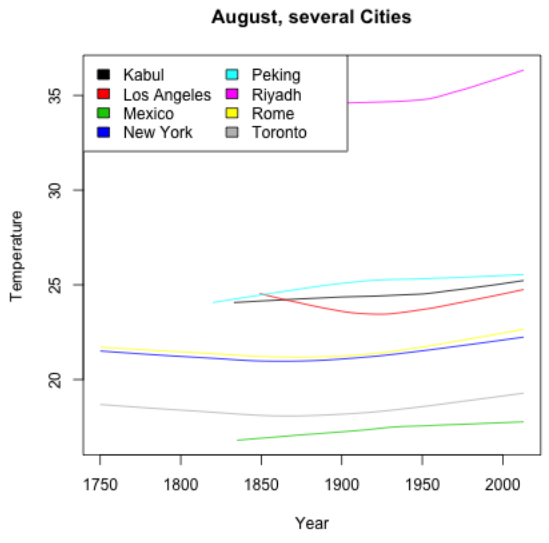
In fact, since it's a bit annoying, I'm going to write a little function to do it.



Look at the code. In what way do they look like t-statistic intervals?

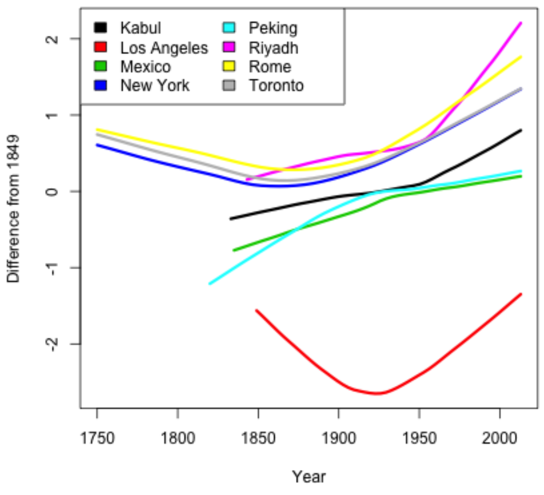
Comparing Many Cities Smooth scatter plots can be useful to compare the time trends of many groups. It's difficult to plot each city, but we can plot their loess curve. I will write a function to automate this. For ease of comparison, I will pick just a few cities in the northern hemisphere.



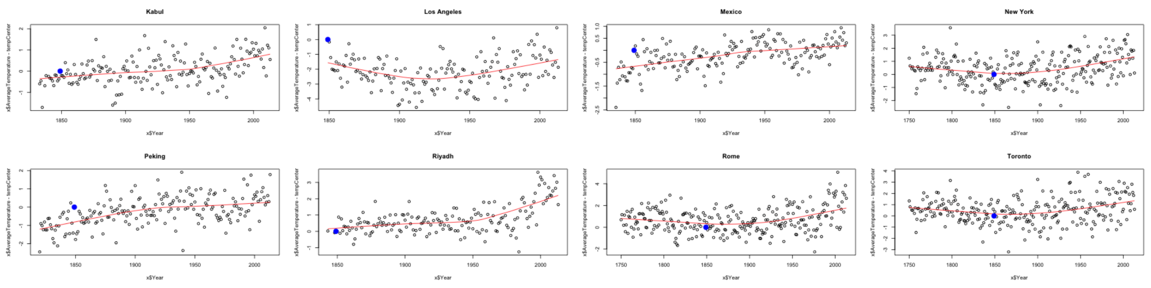


What makes these curves so difficult to compare?

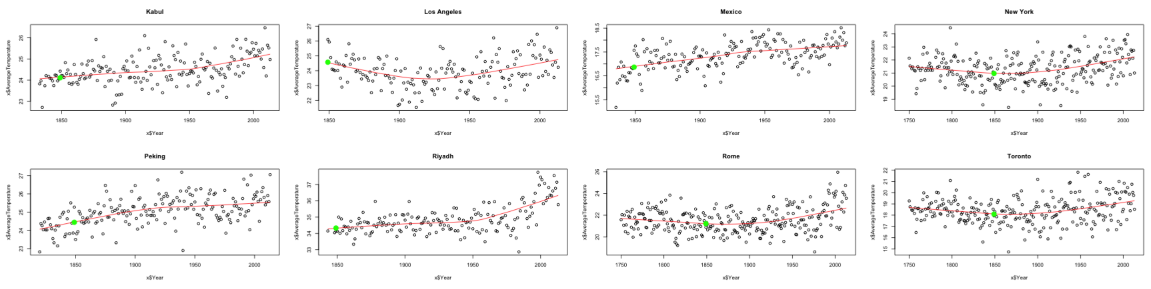
Instead, I'm going to subtract off their temperature in 1849, so that we plot everything relative to that temperature.



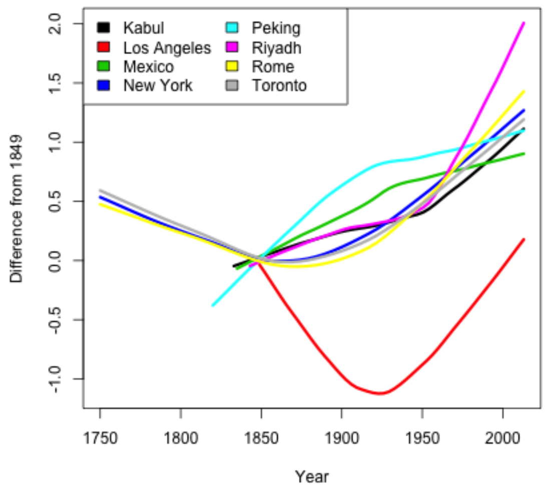
Why don't the curves all go through the same point at 1849? Consider the following plots of the 8 cities, with the 1849 point highlighted in blue.



It would be better to center based on the loess prediction at that point.



Now we can subtract off that value instead.


Kabul
Los Angeles
Mexico
New York
Peking
Riyadh
Rome
Toronto
Difference from 1849
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
1750
1800
1850
1900
1950
2000
Year