Chapter 10

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Quick review of OLS

- OLS stands for "ordinary least-squares".
- Essentially, it means "solve the least-squares problem"

$$\widehat{\beta} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{n} (x_i^{\top} \beta - y_i)^2 = (X^{\top} X)^{-1} X^{\top} Y$$

• The hat matrix is

$$\widehat{Y} = X\widehat{\beta} = X(X^{\top}X)^{-1}X^{\top}Y = HY$$

- The Gauss-Markov theorem says if:
 - 1. $Y_i = x_i^{\top} \beta + \epsilon_i$ 2. $\mathbb{E}\left[\epsilon_i\right] = 0$ 3. $\mathbb{V}\left[\epsilon_i\right] = \sigma^2 < \infty$ 4. $\operatorname{Cov}\left[\epsilon_i, \ \epsilon_j\right] = 0$

Then $\widehat{\beta}$ has the smallest variance of all possible unbiased estimators for β .

What is WLS and why use it?

• Weighted least-squares (WLS) is simply

$$\widehat{\beta} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{n} w_i (x_i^{\top} \beta - y_i)^2 = (X^{\top} W X)^{-1} X^{\top} W Y$$

- If some of those assumptions for G-M are violated, in particular, if $\mathbb{V}\left[\epsilon_{i}\right]$ depends on x_{i} (notated like $\sigma^2(x_i)$, then we lose the optimality.
- Aside: Gauss-Markov is a commonly used justification for OLS in applied work. The logic goes like this: (1) unbiased is good, (2) G-M says OLS is the best linear model which is unbiased. The problem is that (1) is wrong. Unbiased may be good, but often a little bias is better.
- So what does WLS do?
 - 1. It is optimal, in the sense of G-M, if $\mathbb{V}\left[\epsilon_{i}\right] = \sigma_{i}^{2}$.
 - 2. You've already used it (see next slide).
 - 3. What if you want to predict Y_i which have other structures like $y_i \in \{0,1\}$? The algorithms for the new estimators (often called GLS for generalized least squares) use WLS (logistic regression is one example we are building to).

You already used WLS

- I said you already did this. It is convenient that Kernel regression is WLS.
- In particular Kernel regression looks like

$$\widehat{c} = \underset{c}{\operatorname{argmin}} \sum_{i=1}^{n} \sum_{i=1}^{n} w_{ij} (c_j - y_i)^2 \quad w_{ij} = \frac{K((x_i - x_j)/h)}{\sum_{i=1}^{n} K((x_i - x_j)/h)}$$

This is locally constant regression.

You don't need to understand this formula, but it can be useful, and it provides some justification for WLS based on previous ideas.

What goes wrong with heteroskedasticity?

- So suppose $\mathbb{V}[\epsilon_i] = \sigma^2(x_i)$. That is our "homoskedasticity" assumption is violated. Should we care?
- What if we just use OLS (that is lm) anyway?
- Some things don't change.
 - 1. We still have that $\mathbb{E}\left[\widehat{\beta}\right] = \beta$. That is OLS **is** still unbiased.
 - 2. We still have that OLS minimizes the sum of squared residuals: among all lines, OLS makes $\sum_{i=1}^{n} (x_i^{\top} \hat{\beta} - y_i)^2$ as small as possible.
- Some things do change.
 - 1. OLS no longer has the best variance of all unbiased estimators (WLS does).
 - 2. The standard errors that R produces are wrong. They make it seem "more certain" than is correct (could use the bootstrap to fix it though).
 - 3. So are the F-tests and p-values (again, the bootstrap).

Log squared residuals

- So WLS is fairly general. But for now, let's focus on how to use it for heteroskedasticity.
- Suppose you **know** the following:

 - 1. $Y_i=\beta_0+\beta_1X_i+\epsilon_i.$ 2. You know $\beta_0=3$ and $\beta_1=2.$

 - 4. $\mathbb{V}[\epsilon_i] = \sigma^2(x_i)$ ($\sigma^2(\cdot)$ is a function).
- You don't know $\sigma^2(\cdot)$
- How would you estimate $\sigma^2(x)$?
- You can use nonparametric regression of course!
 - Just look at $e_i = y_i 3 + 2x_i$.
 - We already know that e_i has mean zero, so no use estimating it's mean
 - Therefore $\mathbb{E}\left[e_i^2\right] = \sigma^2(x_i)$.
 - Now this is easy: rewrite the model as $e_i^2 = \sigma^2(x_i) + \eta_i$
 - It's just nonparametric regression (since you know e_i^2 and x_i).

So why not?

- There's one problem with the above line of reasoning: $e_i^2 > 0$ so there are some constraints on η_i .
- Imagine if, say, at x=1, $\sigma^2(1)=.001$, then it's pretty likely that η is large and positive there, so there's heteroskedasticity in our model for heteroskedasticity...

- If the original ϵ_i were $N(0, \sigma^2(x_i))$, then the new η_i are distributed as χ_1^2 , so these are right skewed, everywhere.
- A remedy is to look at $\log e_i^2 = \log \sigma^2(x_i) + \tau_i$.
- You could try both and look at qq-plots of the residuals. I tend to prefer the second set-up. It's just more satisfying.
- This is just a transformation: just like when you looked at qq-plots and decided to model $\log Y$ rather than Y.

What's the Oracle?

- So back to WLS.
- I had that example where I wanted to estimate the variance function
- In that case I knew the mean: 3 + 2x
- I knew because the Oracle told me. The Oracle is a wise woman who lives at Delphi according to the ancient Greeks, and speaks the thoughts of Apollo.
- In other words, she tells me things no one could possibly know, like the mean function.
- In statistics, we talk about Oracles a lot, usually as a way of comparing a procedure we cook up for
 estimating something to the answers the Oracle would have told us (the best possible, but unobtainable
 estimator).

A big example

- This is a (slightly modified) portion of a real job interview.
- It is a very simple application of heteroskedasticity.
- Heteroskedasticity appears frequently with financial data, so those companies like to see if you can handle it.

The set up

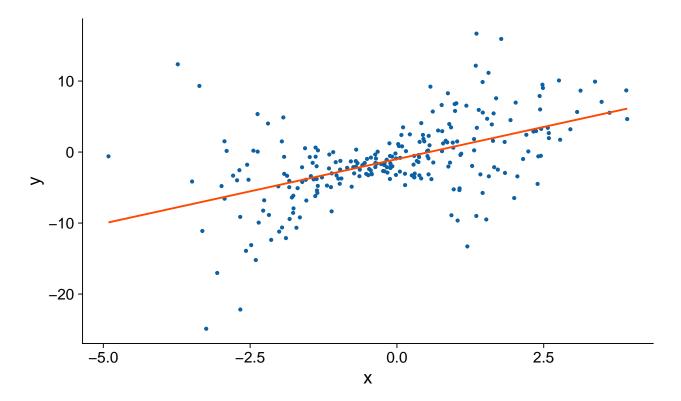
- The dataset jobInt contains data from a simple linear model with heteroskedastic noise.
- In other words, for $i = 1, \ldots, 250$,

$$y_i = \beta_0 + \beta_1 x_i + \sigma(x_i) \epsilon_i$$
 $\epsilon_i \sim N(0, 1).$

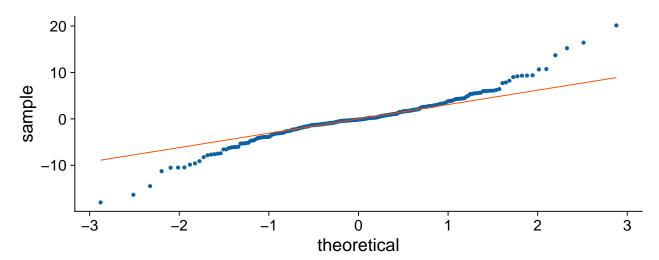
- You know nothing about (the function) $\sigma(\cdot)$.
- Your goal is to estimate (β_0, β_1) as well as possible, and provide a CI.

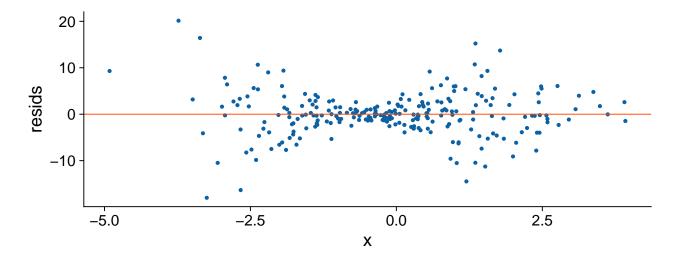
How do I do this?

• First things first, EDA.

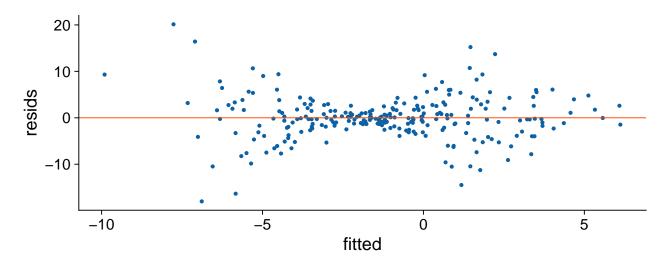


qq-plot and residuals against \mathbf{x}





residuals vs. fitted values



So now what?

- We know that $\mathbb{E}[Y \mid X = x] = \beta_0 + \beta_1 x$.
- We know that $\mathbb{E}\left[\widehat{e} \mid X=x\right]=0$.
- We know that $\mathbb{E}\left[\widehat{e}^2 \mid X = x\right] = \sigma^2(x)$.
- So we want to try to estimate $\sigma^2(x)$ and β_0 and β_1 all at the same time.

Oracle information

- If we knew β_0 and β_1 , then we could use npreg to estimate $\sigma^2(x)$.
- If we knew $\sigma^2(x)$, then we could use WLS to estimate β_0 and β_1 (and all the SEs would be right!)
- But we don't know either.

Procedure

- 1. Use 1m to estimate β_0 and β_1 .
- 2. Now pretend that you "know" them, calculate $\log(\hat{e}^2)$ and use npreg to estimate $\log \sigma^2(x)$.

- 3. Now pretend that you "know" $\sigma^2(x)$ (take exp of your estimate from 2.) and use WLS (with lm(y~x, weights=1/sig2))
- 4. You could stop here. But since you now have "better" estimates of β_1 and β_0 , it's better to iterate 2 and 3 until some convergence.
- 5. Ok. Something converged, so you return the last estimates of β_0 and β_1 . But the SEs are not right (because you "know" $\sigma^2(x)$ but you don't **know** it).
- 6. To get SEs, use the bootstrap:
 - a. Non-parametric: repeat 1-5 B times on resampled data.
 - b. Model-based: this is actually pretty hard here, better not to do it.

Some code

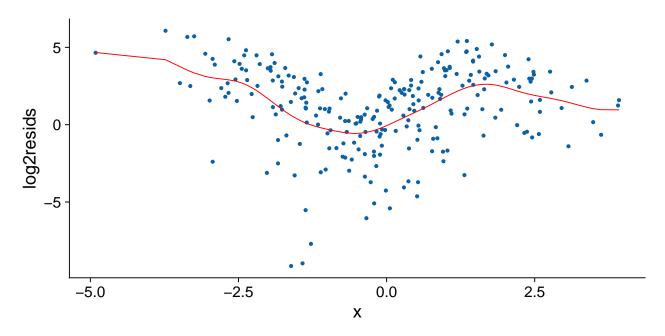
• This code takes in data and does steps 1-5. It is **not** optimized for speed, but for readability, so run with care.

```
heteroWLS <- function(dataFrame, tol = 1e-4, maxit = 100, track=FALSE){
  # inputs: a data object, optional: tolerance, max.iterations, and progress tracker (prints)
  # outputs: estimated betas and weights
  require(np)
  ols = lm(y~x, data=dataFrame)
  b = coefficients(ols)
  conv = FALSE
  for(iter in 1:maxit){ # don't let this run forever
    if(conv) break # if the b's stop moving, get out of the loop
   logSqResids = log(residuals(ols)^2)
   winv = exp(predict(npreg(logSqResids~x, data=dataFrame, tol=1e-2, ftol=1e-2)))
   winv[winv < tol] = tol # zero inverse weights are bad, make them small
   ols = lm(y~x, weights = 1/winv, data=dataFrame) #weights are 1 / estim.variance
   newb = coefficients(ols)
    conv.crit = sum((b-newb)^2) # calculate how much b moved
   if(track) cat('\n', iter, '/', maxit, ' conv.crit = ', conv.crit) # print progress
   conv = (conv.crit < tol) # check if the b's changed much</pre>
   b = newb # update the coefficient estimates
  }
  return(list(betas=b, weights = winv, log2resids = log(residuals(ols)^2)))
}
```

Do it! (takes a little while...)

```
resampWLS <- function(dataFrame,...){ # ... means options passed on
  rowSamp = sample(1:nrow(dataFrame), size=nrow(dataFrame), replace=TRUE)
  return(heteroWLS(dataFrame[rowSamp,],...)$betas) # passed things on if desired
}
B = 100 #
alp = .05
origBetas = heteroWLS(jobInt)
system.time(bootBetas <- replicate(B, resampWLS(jobInt, maxit=20)))</pre>
qq = apply(bootBetas, 1, quantile, probs=c(1-alp/2, alp/2))
CI = cbind(origBetas$betas, 2*origBetas$betas - t(qq))
colnames(CI) = c('coef', rev(colnames(CI)[2:3]))
##
                               2.5%
                                          97.5%
                     coef
## (Intercept) -0.9938074 -1.406956 -0.4306921
## x
                2.0023640 1.607402 2.6352379
```

Some plots



Some caveats

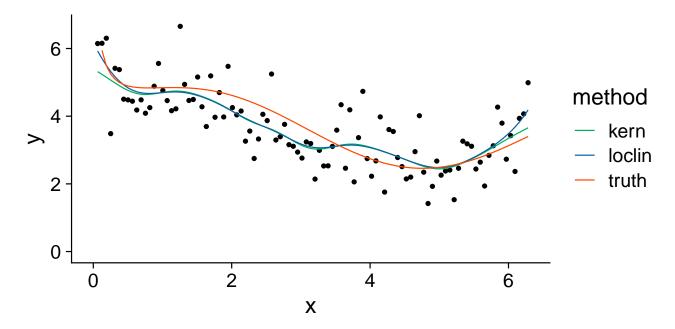
- If we care about estimating $\sigma(\cdot)$, then what we did is ok.
- But we don't.
- We only care about estimating β_0 and β_1 .
- So better to use CV with leaving out (y_i, x_i) , instead of using CV to estimate $\sigma(\cdot)$ (which is what npreg is doing; it knows nothing about y_i)
- This takes a bit more work to code up (Try it!)

Local linear vs. Kernels

- People often wonder whether to use local linear regression or Kernels.
- Like with many things, there isn't really a cut-and-dried answer.
- Some practitioners prefer local linear regression.
- It's main benefit is to correct "boundary bias".
- Otherwise, not much different.

Repeat of Ch. 4

• We can estimate this easily with both a kernel and local linear regression



What is Loess?

- So kernel regressions are local constants, we then saw local linear regression which is quite similar.
- Why stop there? The next term is squared things, then cubics, then...
- Loess uses local polynomials (of some order) in a particular way (combining k-nearest neighbor regression with subsampling).
- It is actually quite cool, but it's complexity makes it hard to deal with.
- Theoretically, one can show that Kernels are optimal, so it's not really worth worrying too much about, but it can work well, and it doesn't require installing a package.
- Here it is on my previous example

