Date Science with R and Python

Statistical models

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Agenda

- Using data frames for statistical purposes
- Manipulation of data into more convenient forms
- (Re-)Introduction to linear models and the model space

So You've Got A Data Frame. What can we do with it?

- Plot it: examine multiple variables and distributions
- Test it: compare groups of individuals to each other
- Check it: does it conform to what we'd like for our needs?

Test Case: Birth weight data

Included in R already:

```
library(tidyverse)
library(lubridate)
library(MASS)
data(birthwt)
summary(birthwt)
```

```
##       low              age              lwt              race      
##  Min.   :0.0000   Min.   :14.00   Min.   : 80.0   Min.   :1.000  
##  1st Qu.:0.0000   1st Qu.:19.00   1st Qu.:110.0   1st Qu.:1.000  
##  Median :0.0000   Median :23.00   Median :121.0   Median :1.000  
##  Mean   :0.3122   Mean   :23.24   Mean   :129.8   Mean   :1.847  
##  3rd Qu.:1.0000   3rd Qu.:26.00   3rd Qu.:140.0   3rd Qu.:3.000  
##  Max.   :1.0000   Max.   :45.00   Max.   :250.0   Max.   :3.000  
##      smoke            ptl               ht                ui        
##  Min.   :0.0000   Min.   :0.0000   Min.   :0.00000   Min.   :0.0000  
##  1st Qu.:0.0000   1st Qu.:0.0000   1st Qu.:0.00000   1st Qu.:0.0000  
##  Median :0.0000   Median :0.0000   Median :0.00000   Median :0.0000  
##  Mean   :0.3915   Mean   :0.1958   Mean   :0.06349   Mean   :0.1481  
##  3rd Qu.:1.0000   3rd Qu.:0.0000   3rd Qu.:0.00000   3rd Qu.:0.0000  
##  Max.   :1.0000   Max.   :3.0000   Max.   :1.00000   Max.   :1.0000  
##       ftv              bwt          
##  Min.   :0.0000   Min.   : 709   
```

Make it readable!

```
colnames(birthwt)
```

```
##  [1] "low"   "age"   "lwt"   "race"  "smoke" "ptl"   "ht"    "ui"    "ftv"
## [10] "bwt"
```

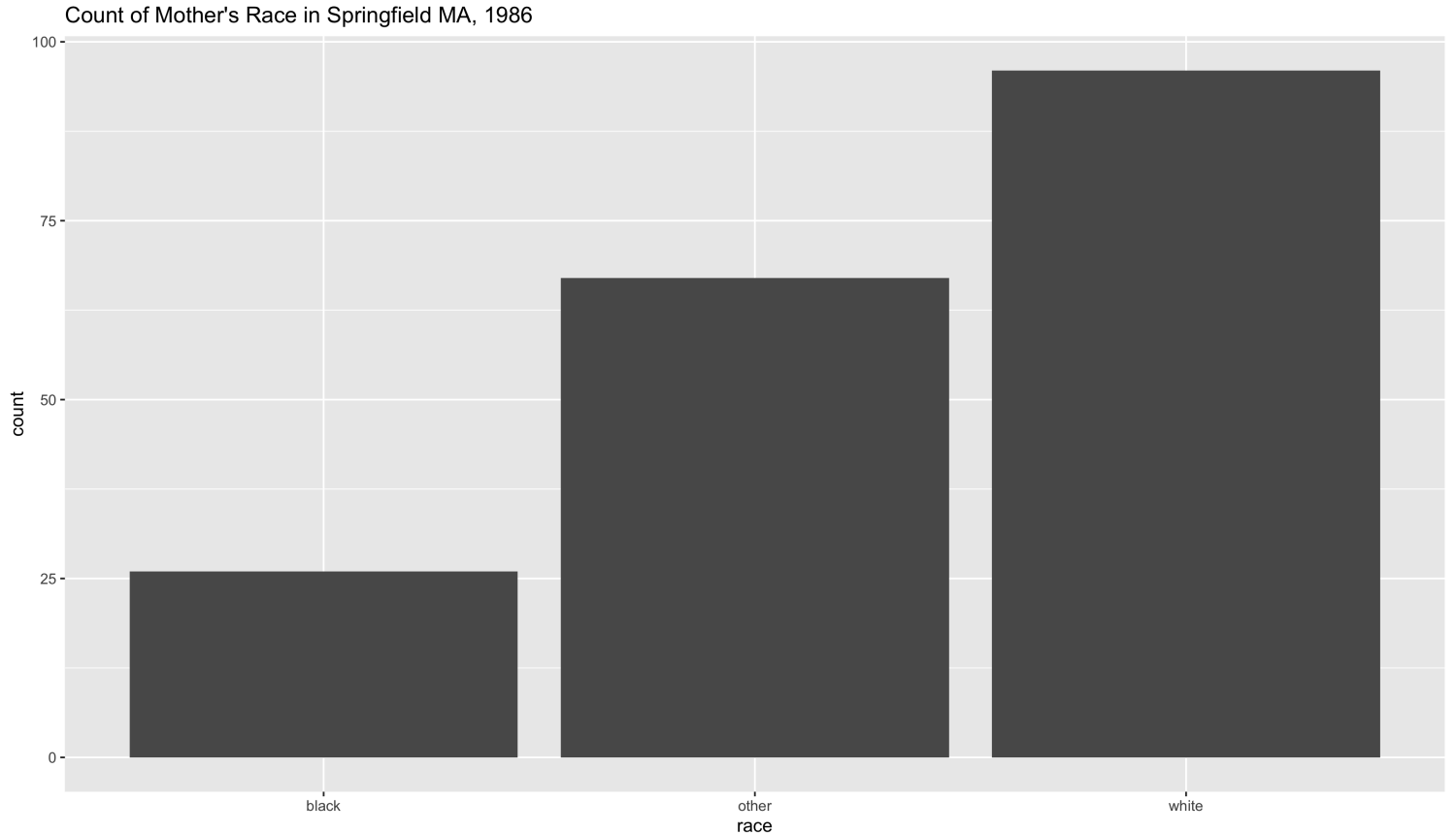
```
colnames(birthwt) <- c("birthwt.below.2500", "mother.age",
                       "mother.weight", "race",
                       "mother.smokes", "previous.prem.labor",
                       "hypertension", "uterine.irr",
                       "physician.visits", "birthwt.grams")
```

Let's make all the factors more descriptive.

```
birthwt$race <- factor(c("white", "black", "other")[birthwt$race])
birthwt$mother.smokes <- factor(c("No", "Yes")[birthwt$mother.smokes
birthwt$uterine.irr <- factor(c("No", "Yes")[birthwt$uterine.irr + 1]
birthwt$hypertension <- factor(c("No", "Yes")[birthwt$hypertension +
```

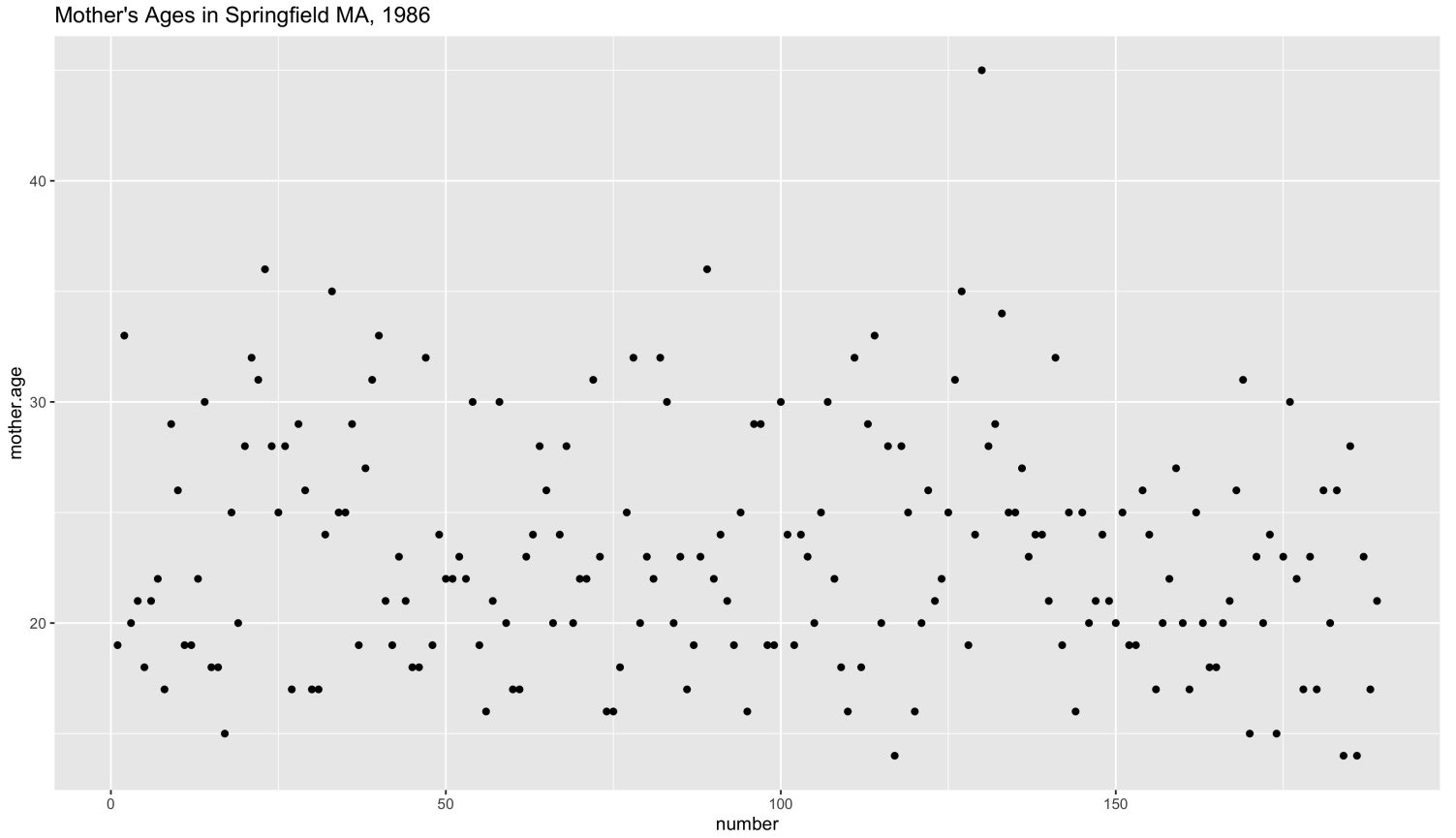
Bar plot for race

```
birthwt %>% ggplot(aes(x = race))+
  geom_bar()+
  labs(title = "Count of Mother's Race in Springfield MA, 1986")
```



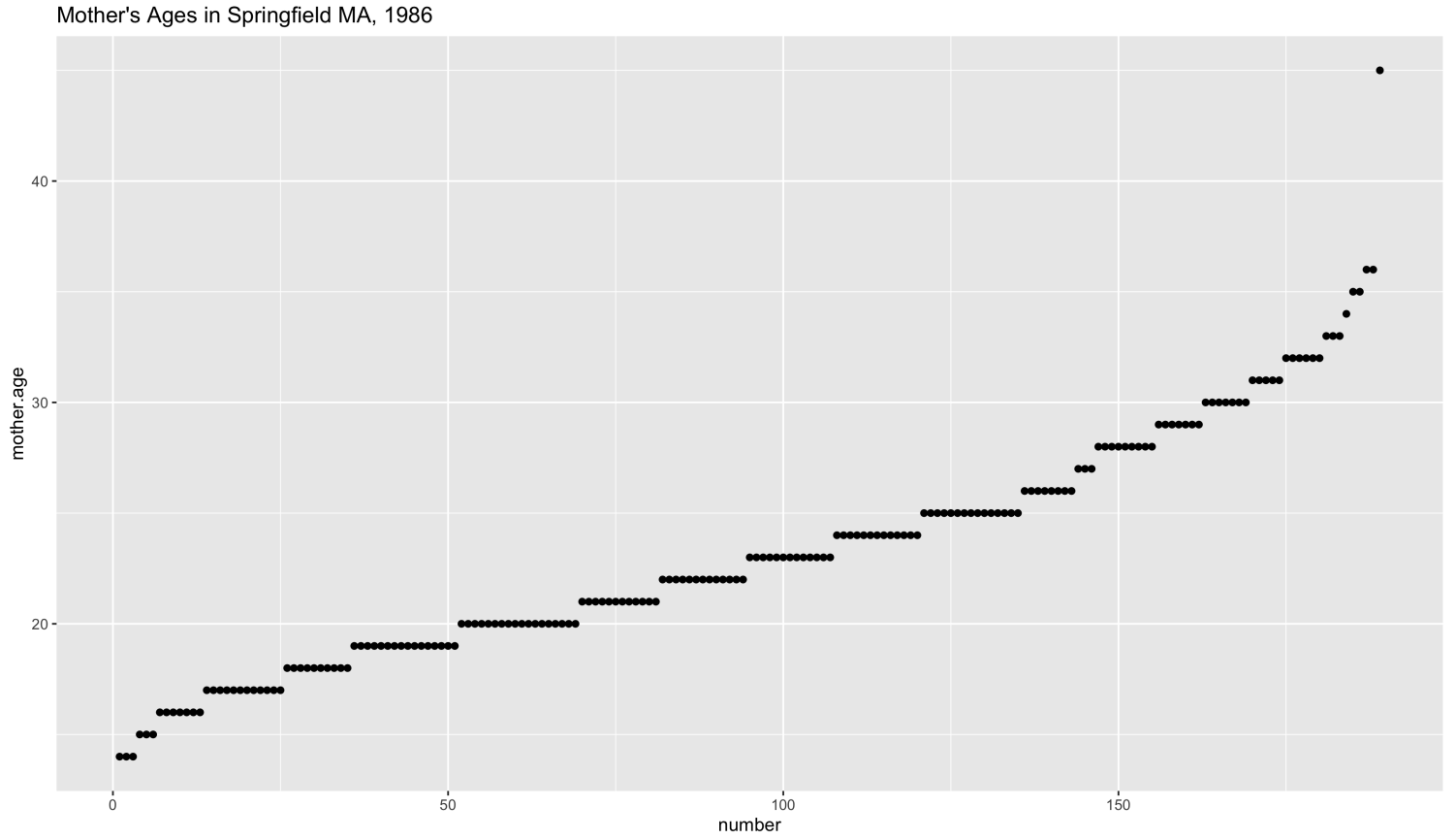
Scatter plot for mother's ages

```
birthwt %>% ggplot(aes(x = 1:nrow(birthwt), y = mother.age))+
  geom_point()+
  labs(x = 'number', title = "Mother's Ages in Springfield MA, 1986")
```



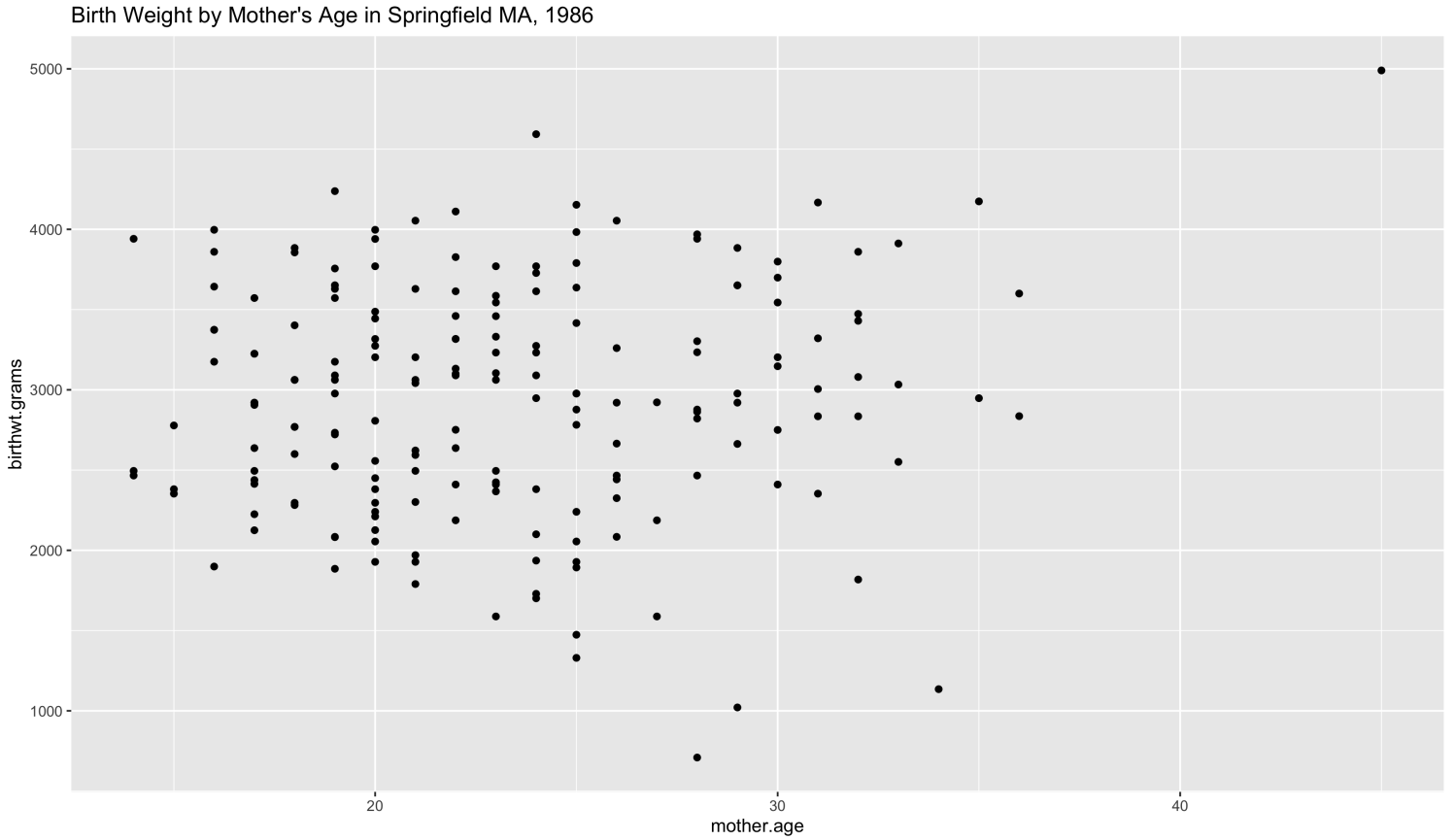
Sorted mother's ages

```
birthwt %>% arrange(mother.age) %>% ggplot(aes(x = 1:nrow(birthwt), y
  geom_point()+
  labs(x = 'number', title = "Mother's Ages in Springfield MA, 1986")
```



Birth weight versus mother's ages

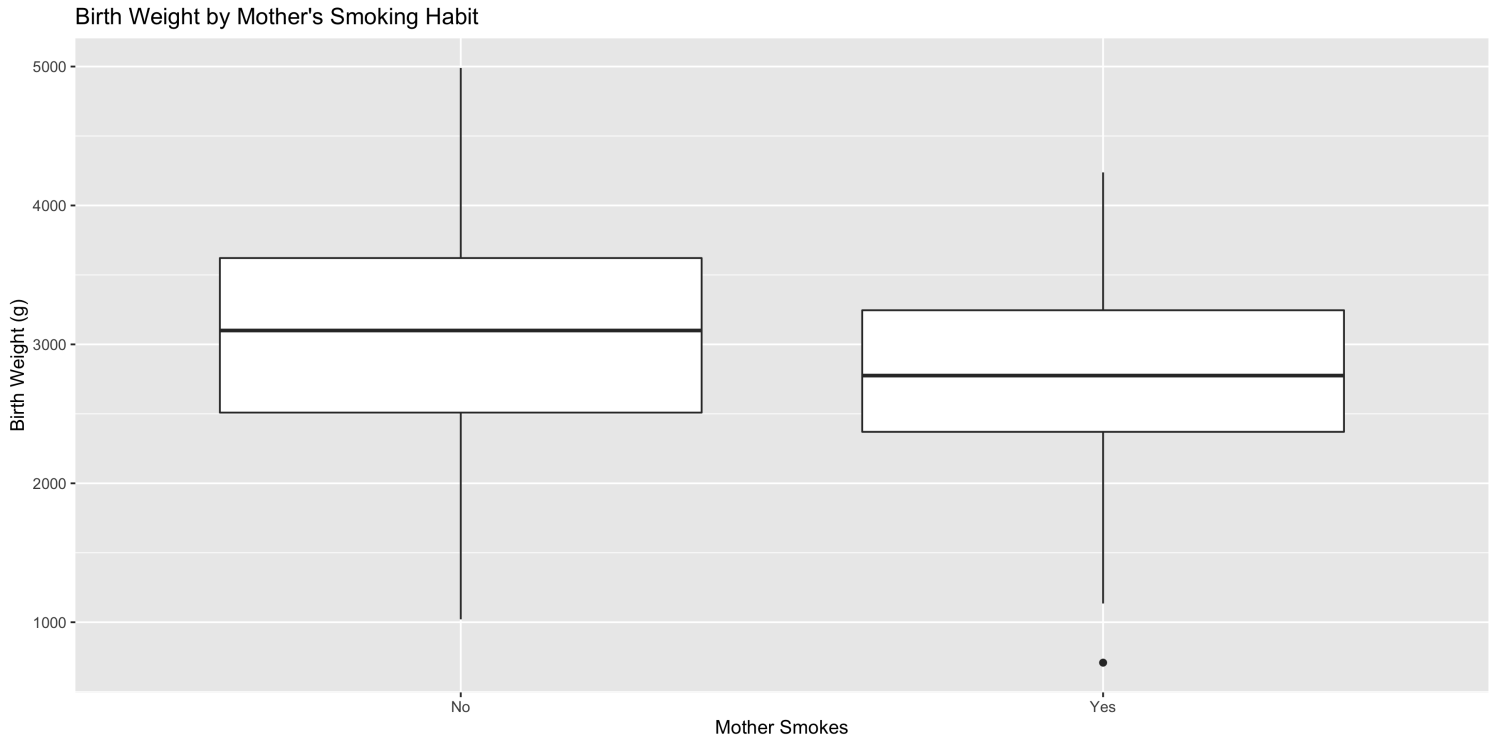
```
birthwt %>% ggplot(aes(x = mother.age, y = birthwt.grams))+
  geom_point()+
  labs(title = "Birth Weight by Mother's Age in Springfield MA, 1986"
```



Boxplot

Let's fit some models to the data pertaining to our outcome(s) of interest.

```
birthwt %>% ggplot(aes(x = mother.smokes, y = birthwt.grams))+
  geom_boxplot()+
  labs(title = "Birth Weight by Mother's Smoking Habit", y = "Birth W
```



Basic statistical testing

Tough to tell! Simple two-sample t-test:

```
t.test (birthwt$birthwt.grams[birthwt$mother.smokes == "Yes"],
        birthwt$birthwt.grams[birthwt$mother.smokes == "No"]) #, var
```

```
##
##     Welch Two Sample t-test
##
## data:  birthwt$birthwt.grams[birthwt$mother.smokes == "Yes"] and birthwt$b
## t = -2.7299, df = 170.1, p-value = 0.007003
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
##  -488.97860  -78.57486
## sample estimates:
## mean of x mean of y
##  2771.919  3055.696
```

Does this difference match the linear model?

```
linear.model.1 <- lm (birthwt.grams ~ mother.smokes, data=birthwt)
summary(linear.model.1)
```

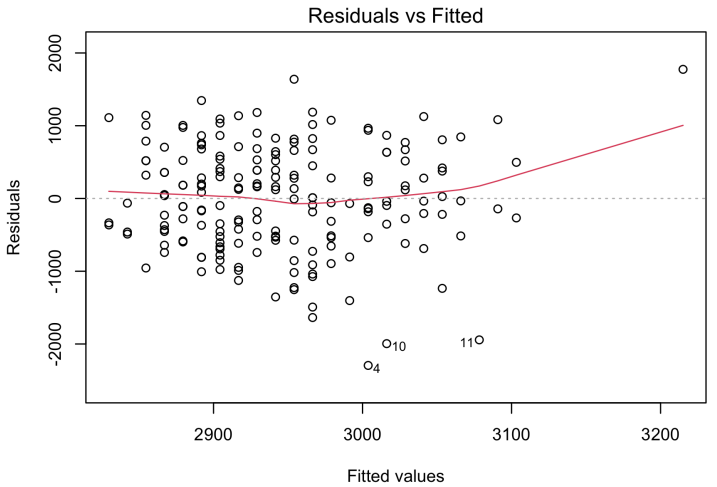
```
##
## Call:
## lm(formula = birthwt.grams ~ mother.smokes, data = birthwt)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2062.9  -475.9    34.3   545.1  1934.3
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)       3055.70      66.93  45.653  < 2e-16 ***
## mother.smokesYes  -283.78     106.97  -2.653  0.00867 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 717.8 on 187 degrees of freedom
## Multiple R-squared:  0.03627,    Adjusted R-squared:  0.03112
## F-statistic: 7.038 on 1 and 187 DF,  p-value: 0.008667
```

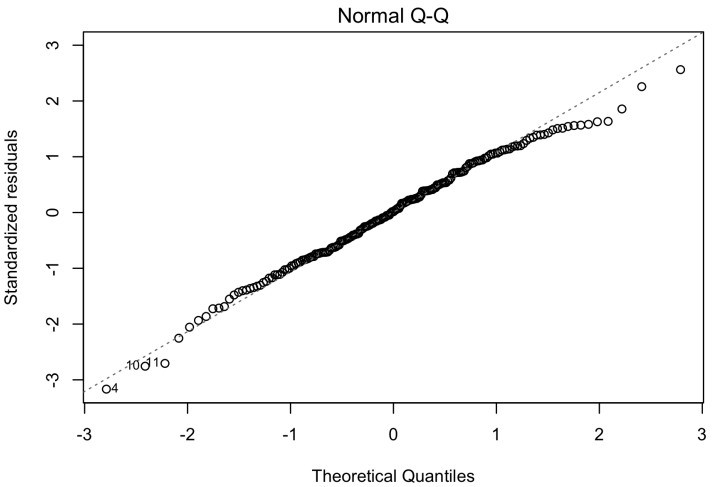
Basic statistical testing

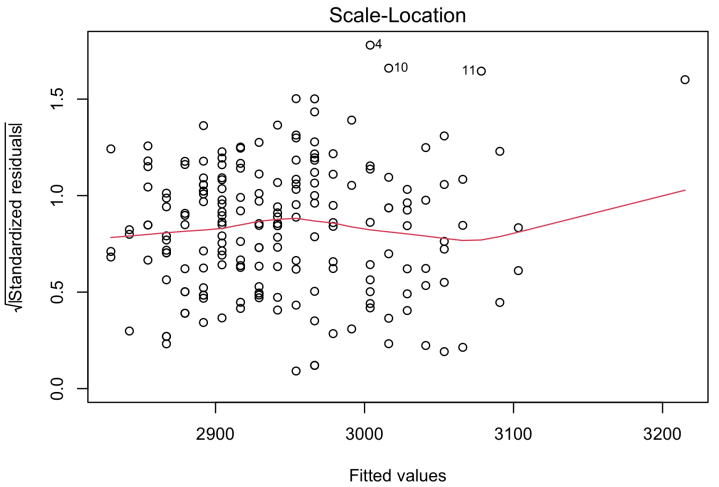
Does this difference match the linear model?

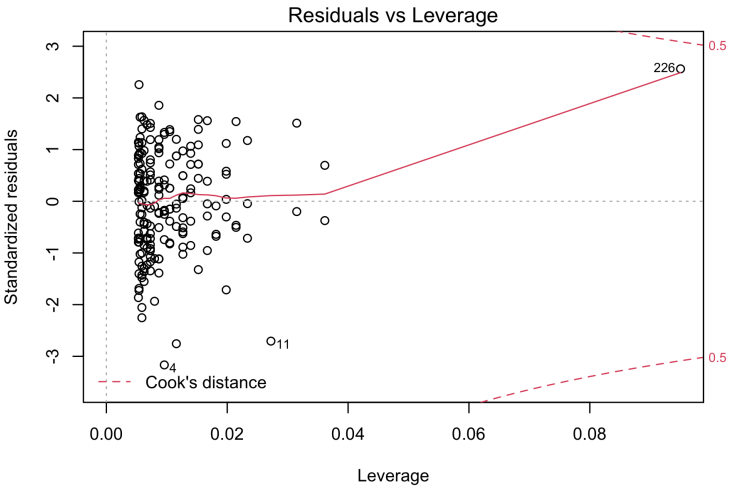
```
linear.model.2 <- lm (birthwt.grams ~ mother.age, data=birthwt)
summary(linear.model.2)
```

```
##
## Call:
## lm(formula = birthwt.grams ~ mother.age, data = birthwt)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2294.78  -517.63    10.51   530.80  1774.92
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  2655.74     238.86   11.12   <2e-16 ***
## mother.age     12.43      10.02    1.24    0.216
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 728.2 on 187 degrees of freedom
## Multiple R-squared:  0.008157,    Adjusted R-squared:  0.002853
## F-statistic: 1.538 on 1 and 187 DF,  p-value: 0.2165
```


Residuals vs Fitted
Residuals
Fitted values
2900
3000
3100
3200
-2000
-1000
0
1000
2000
10
11
4


Normal Q-Q
Standardized residuals
Theoretical Quantiles
-3
-2
-1
0
1
2
3
10
1
4


Scale-Location
√|Standardized residuals|
Fitted values
2900
3000
3100
3200
0.0
0.5
1.0
1.5
4
10
11


Residuals vs Leverage
Standardized residuals
Leverage
0.00
0.02
0.04
0.06
0.08
-3
-2
-1
0
1
2
3
0.5
0.5
226
11
4
Cook's distance

Detecting Outliers

These are the default diagnostic plots for the analysis. Note that our oldest mother and her heaviest child are greatly skewing this analysis as we suspected.

```
birthwt.noout <- birthwt %>% filter(mother.age <= 40)
linear.model.3 <- lm (birthwt.grams ~ mother.age, data=birthwt.noout)
summary(linear.model.3)
```

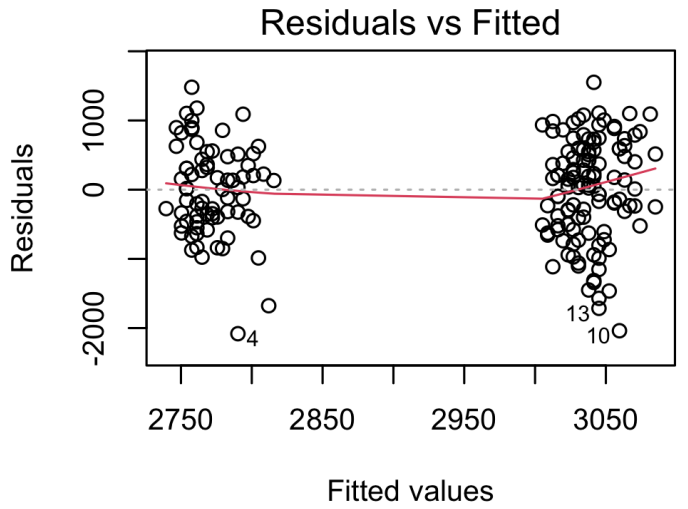
```
##
## Call:
## lm(formula = birthwt.grams ~ mother.age, data = birthwt.noout)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2245.89  -511.24    26.45   540.09  1655.48
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 2833.273    244.954   11.57   <2e-16 ***
## mother.age     4.344     10.349    0.42    0.675
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 717.2 on 186 degrees of freedom
```

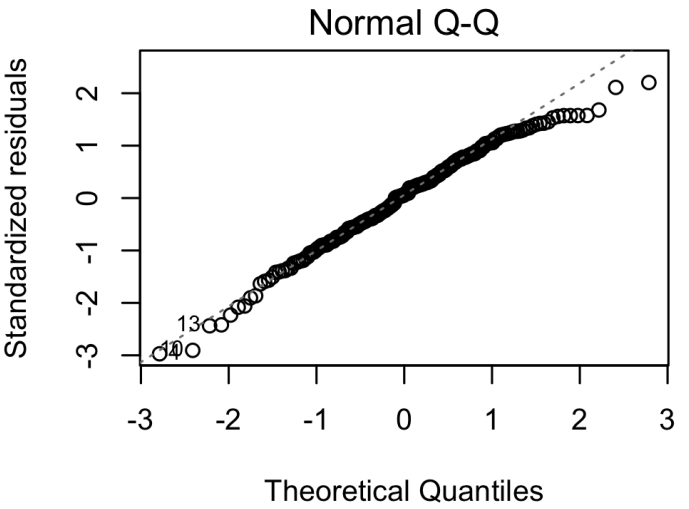
More complex models

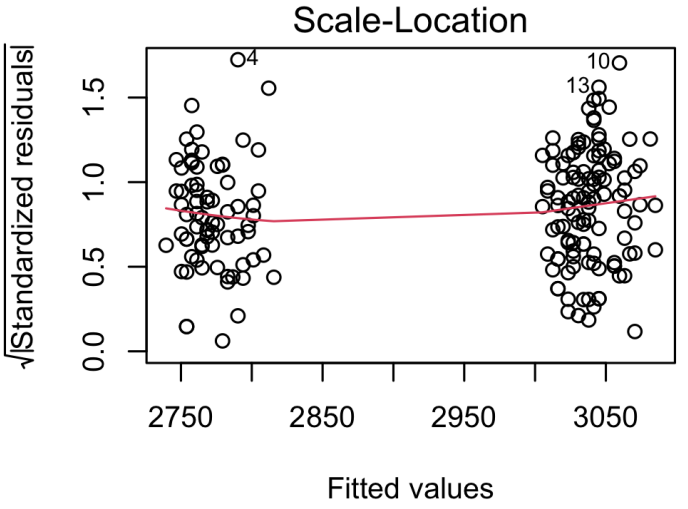
Add in smoking behavior:

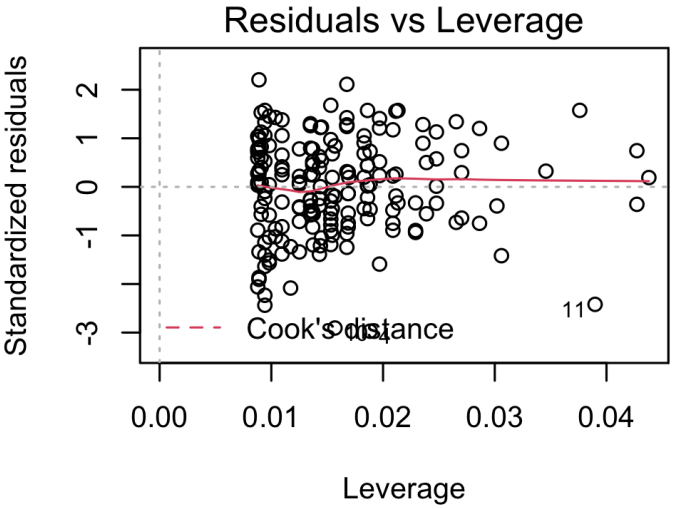
```
linear.model.3a <- lm (birthwt.grams ~ + mother.smokes + mother.age,
summary(linear.model.3a)
```

```
##
## Call:
## lm(formula = birthwt.grams ~ +mother.smokes + mother.age, data = birthwt.r
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2081.22  -459.82    43.56   548.22  1551.51
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)       2954.582    246.280  11.997   <2e-16 ***
## mother.smokesYes -265.756    105.605  -2.517   0.0127 *
## mother.age          3.621     10.208   0.355   0.7232
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 707.1 on 185 degrees of freedom
## Multiple R-squared:  0.03401,    Adjusted R-squared:  0.02357
## F-statistic: 3.257 on 2 and 185 DF,  p-value: 0.04072
```


Residuals vs Fitted
Residuals
Fitted values
2750
2850
2950
3050
-2000
0
1000
4
13
10


Normal Q-Q
Standardized residuals
Theoretical Quantiles
-3
-2
-1
0
1
2
3
13


Scale-Location
√|Standardized residuals|
Fitted values
2750
2850
2950
3050
0.0
0.5
1.0
1.5
4
10
13

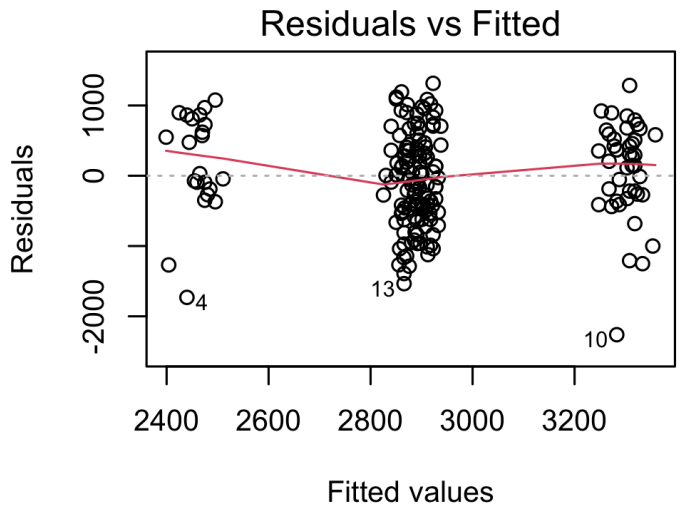

Residuals vs Leverage
Standardized residuals
Leverage
0.00
0.01
0.02
0.03
0.04
-3
-1
0
1
2
Cook's distance
11

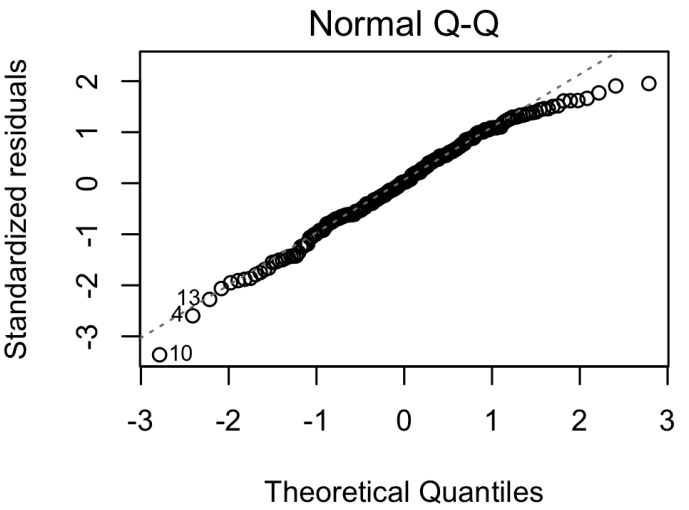
More complex models

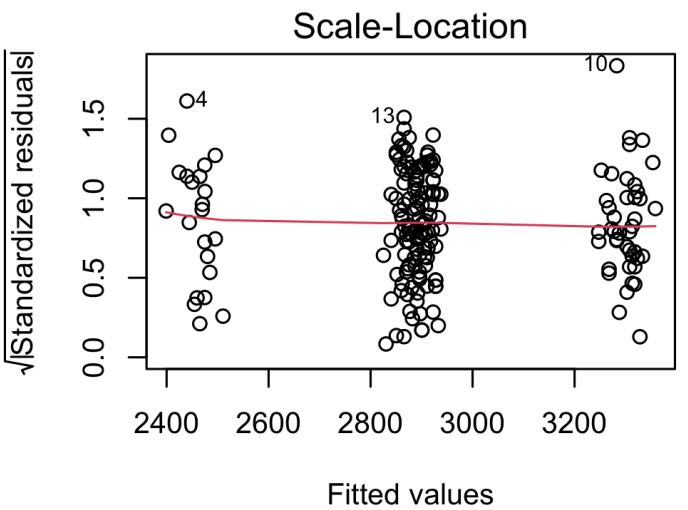
Add in smoking behavior:

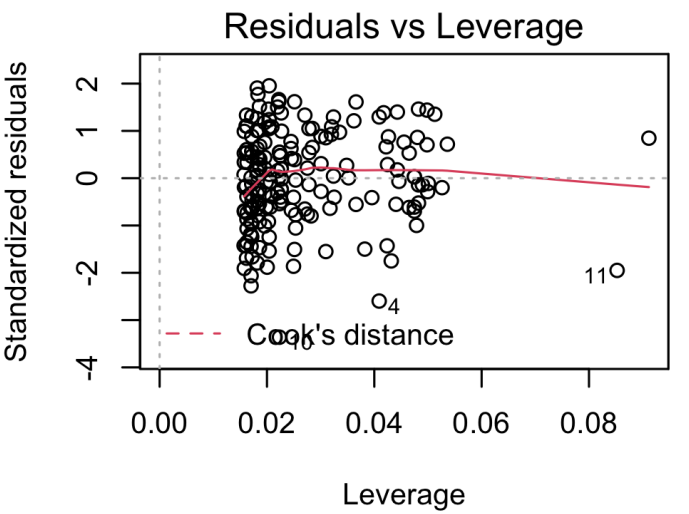
```
linear.model.3b <- lm (birthwt.grams ~ mother.age + mother.smokes + r
summary(linear.model.3b)
```

```
##
## Call:
## lm(formula = birthwt.grams ~ mother.age + mother.smokes + race,
##     data = birthwt.noout)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2261.76  -422.49    15.98   512.00  1315.40
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)       2986.405    260.897  11.447  < 2e-16 ***
## mother.age          -5.050     10.056  -0.502 0.616136
## mother.smokesYes  -410.656    108.635  -3.780 0.000212 ***
## raceother            5.487    158.918   0.035 0.972492
## racewhite          442.799    154.023   2.875 0.004521 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```


Residuals vs Fitted
Residuals
Fitted values
4
13
10


Normal Q-Q
Standardized residuals
Theoretical Quantiles
13
4
10


Scale-Location
√|Standardized residuals|
Fitted values
4
13
10


Residuals vs Leverage
Standardized residuals
Leverage
Cook's distance
4
11

Everything Must Go (In)

Let's do a kitchen sink model on this new data set:

```
linear.model.4 <- lm (birthwt.grams ~ ., data=birthwt.noout)
summary(linear.model.4)
```

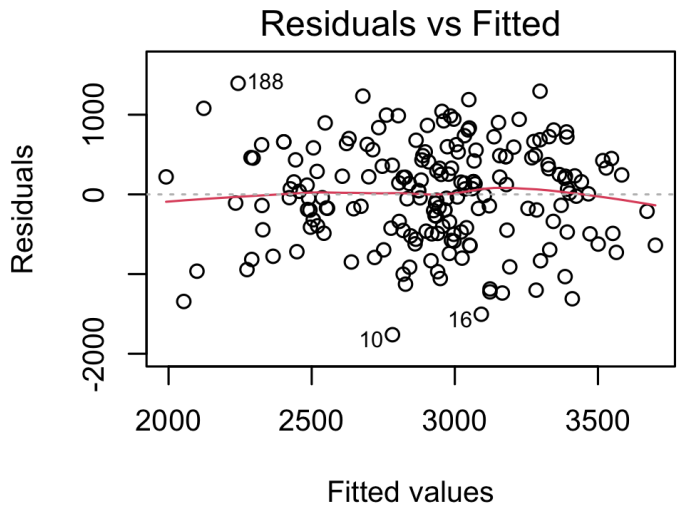
```
##
## Call:
## lm(formula = birthwt.grams ~ ., data = birthwt.noout)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -985.04 -274.13  -13.87  262.53 1146.50
##
## Coefficients:
##                       Estimate Std. Error t value Pr(>|t|)
## (Intercept)          3360.5163   215.4112  15.600  < 2e-16 ***
## birthwt.below.2500  -1116.3933    70.8578 -15.755  < 2e-16 ***
## mother.age            -16.0321     6.4159  -2.499 0.013373 *
## mother.weight           1.9317     1.1208   1.723 0.086545 .
## raceother              68.8145   101.4451   0.678 0.498441
## racewhite             247.0241    96.4935   2.560 0.011302 *
## mother.smokesYes     -157.7041    68.6205  -2.298 0.022719 *
## previous.prem.labor    95.9825    65.3329   1.469 0.143573
## hypertensionYes      -185.2778   131.0126  -1.414 0.159060
```

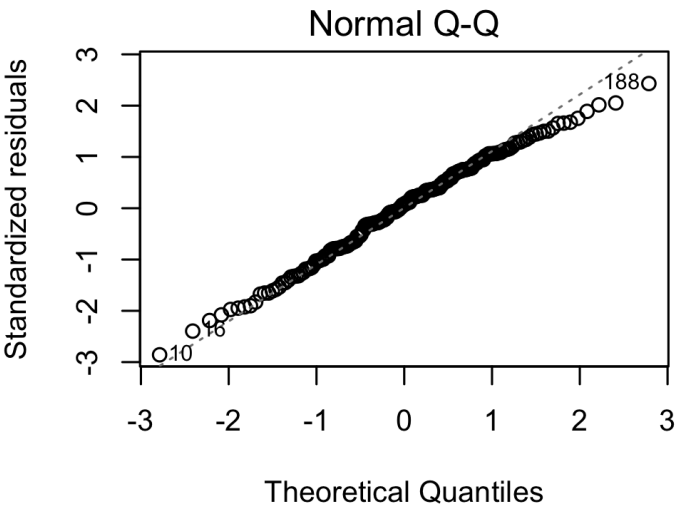
Everything Must Go (In), Except What Must Not

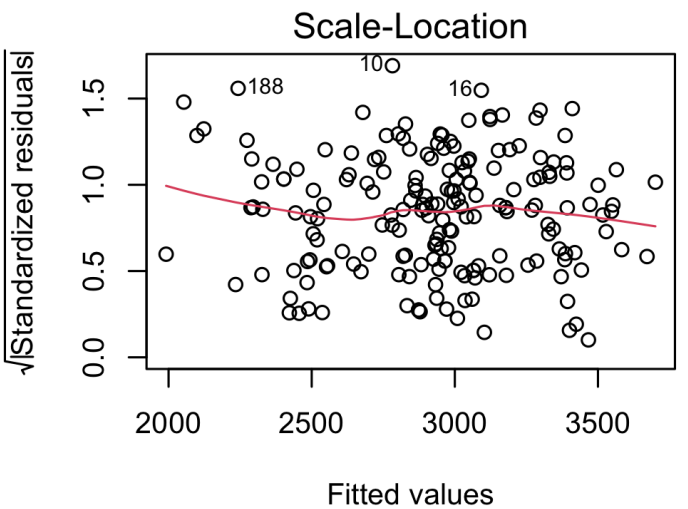
Whoops! One of those variables was `birthwt.below.2500` which is a function of the outcome.

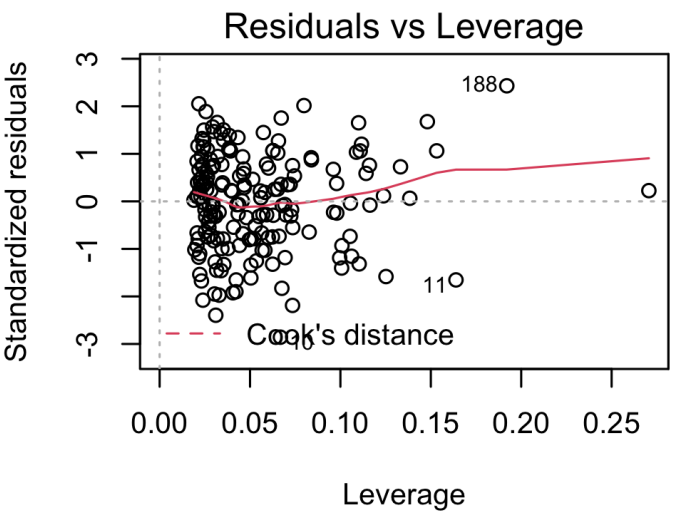
```
linear.model.4a <- lm (birthwt.grams ~ . - birthwt.below.2500, data=b
summary(linear.model.4a)
```

```
##
## Call:
## lm(formula = birthwt.grams ~ . - birthwt.below.2500, data = birthwt.noout)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1761.10  -454.81    46.43   459.78  1394.13
##
## Coefficients:
##                    Estimate Std. Error t value Pr(>|t|)
## (Intercept)        2545.584    323.204   7.876 3.21e-13 ***
## mother.age          -12.111      9.909  -1.222 0.223243
## mother.weight         4.789      1.710   2.801 0.005656 **
## raceother           155.605    156.564   0.994 0.321634
## racewhite           494.545    147.153   3.361 0.000951 ***
## mother.smokesYes   -335.793    104.613  -3.210 0.001576 **
## previous.prem.labor  -32.922    100.185  -0.329 0.742838
## hypertensionYes     -594.324    198.480  -2.994 0.003142 **
```


Residuals vs Fitted
Residuals
Fitted values
188
10
16
-2000
0
1000
2000
2500
3000
3500


Normal Q-Q
Standardized residuals
Theoretical Quantiles
188
16
10
-3
-2
-1
0
1
2
3

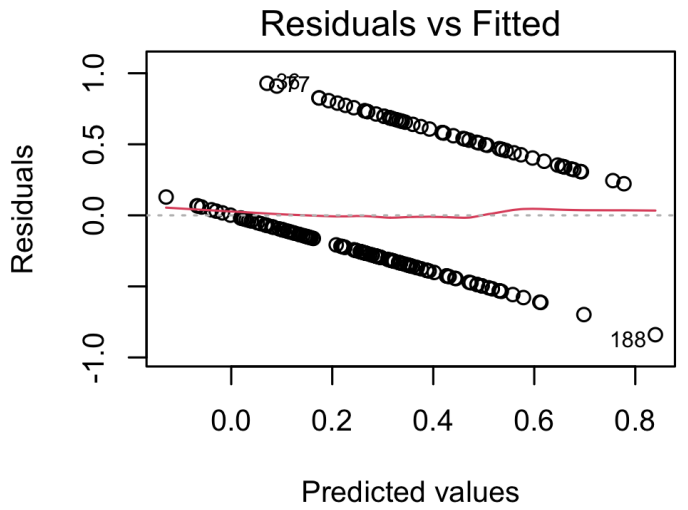

Scale-Location
√|Standardized residuals|
Fitted values
188
10
16
0.0
0.5
1.0
1.5
2000
2500
3000
3500

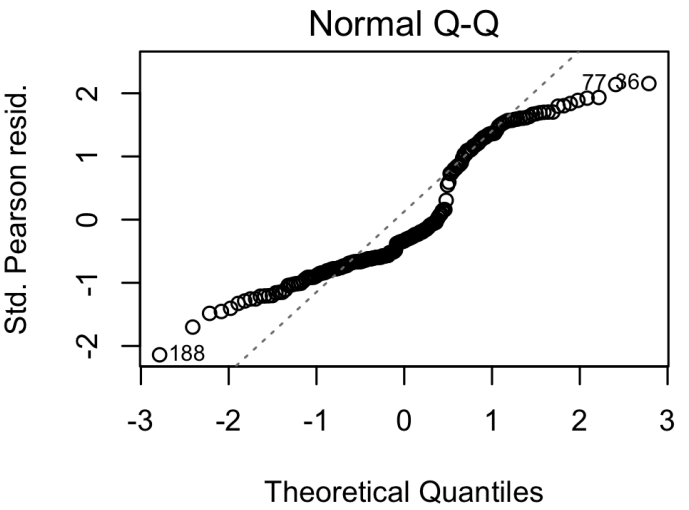

Residuals vs Leverage
Standardized residuals
Leverage
188
11
16
Cook's distance
-3
-1
0
1
2
3
0.00
0.05
0.10
0.15
0.20
0.25

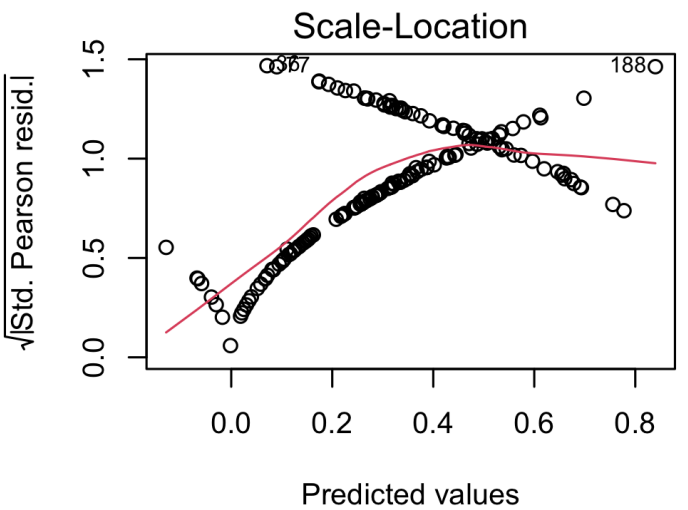
Generalized Linear Models

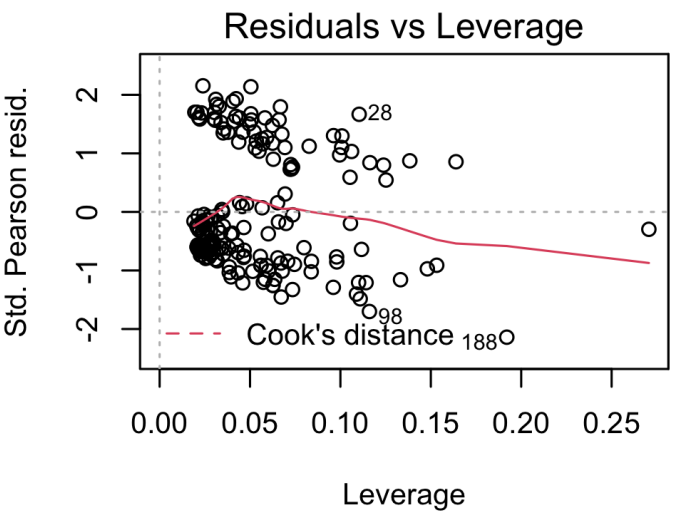
Maybe a linear increase in birth weight is less important than if it's below a threshold like 2500 grams (5.5 pounds). Let's fit a generalized linear model instead:

```
glm.0 <- glm (birthwt.below.2500 ~ . - birthwt.grams, data=birthwt.nc
```


Residuals vs Fitted
Residuals
Predicted values
367
188
1.0
0.5
0.0
-1.0
0.0
0.2
0.4
0.6
0.8


Normal Q-Q
Std. Pearson resid.
Theoretical Quantiles
77
36
188
2
1
0
-1
-2
-3
-2
-1
0
1
2
3


Scale-Location
√|Std. Pearson resid.|
Predicted values
367
188
1.5
1.0
0.5
0.0
0.0
0.2
0.4
0.6
0.8

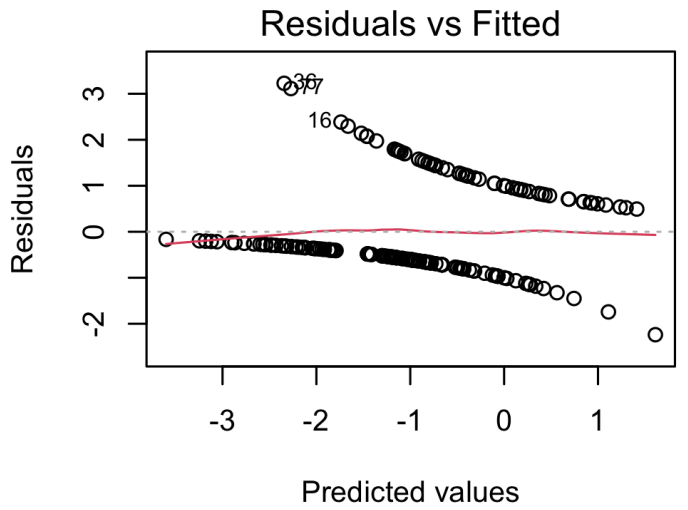

Residuals vs Leverage
Std. Pearson resid.
Leverage
28
98
188
Cook's distance
2
1
0
-1
-2
0.00
0.05
0.10
0.15
0.20
0.25

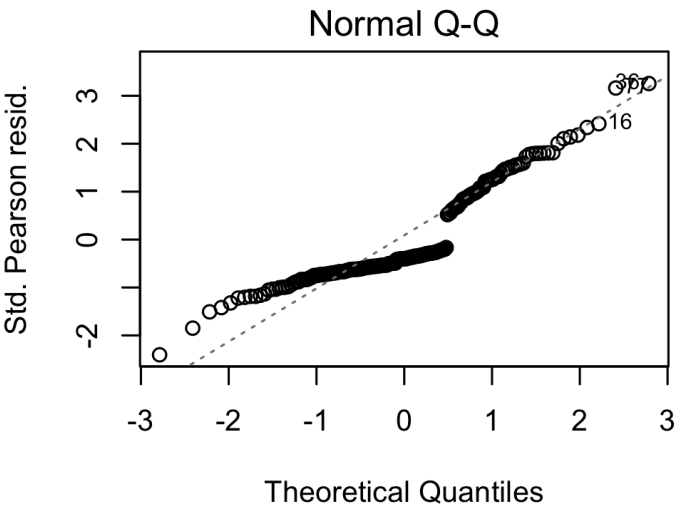
Generalized Linear Models

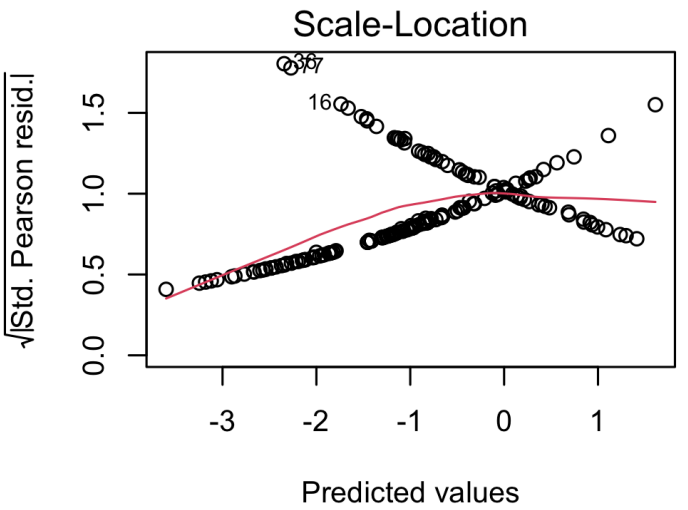
The default value is a Gaussian model (a standard linear model). Change this:

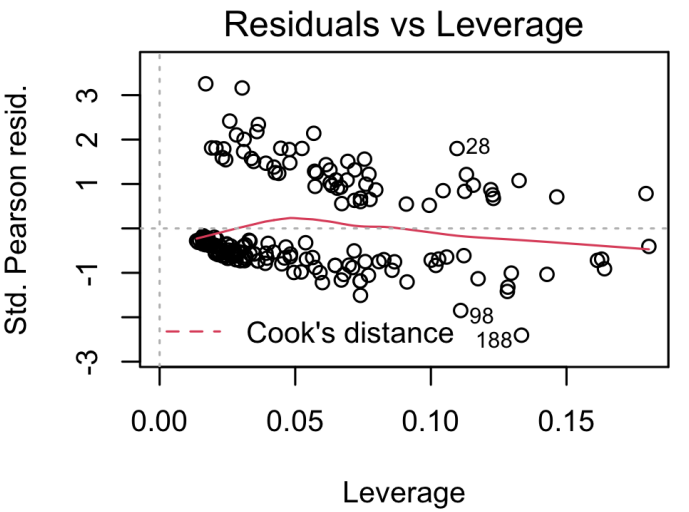
```
glm.1 <- glm (birthwt.below.2500 ~ . - birthwt.grams, data=birthwt.nc
summary(glm.1)
```

```
##
## Call:
## glm(formula = birthwt.below.2500 ~ . - birthwt.grams, family = binomial(li
##     data = birthwt.noout)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -1.8938  -0.8222  -0.5363   0.9848   2.2069
##
## Coefficients:
##                      Estimate Std. Error z value Pr(>|z|)
## (Intercept)          1.721830   1.258897   1.368  0.17140
## mother.age          -0.027537   0.037718  -0.730  0.46534
## mother.weight       -0.015474   0.006919  -2.237  0.02532 *
## raceother           -0.395505   0.537685  -0.736  0.46199
## racewhite           -1.269006   0.527180  -2.407  0.01608 *
## mother.smokesYes     0.931733   0.402359   2.316  0.02058 *
## previous.prem.labor  0.539549   0.345413   1.562  0.11828
## hypertensionYes      1.860521   0.697502   2.667  0.00764 **
```


Residuals vs Fitted
Residuals
Predicted values
367
16


Normal Q-Q
Std. Pearson resid.
Theoretical Quantiles
367
16


Scale-Location
√|Std. Pearson resid.|
Predicted values
367
16


Residuals vs Leverage
Std. Pearson resid.
Leverage
Cook's distance
28
98
188

What Do We Do With This, Anyway?

Let's take a subset of this data to do predictions.

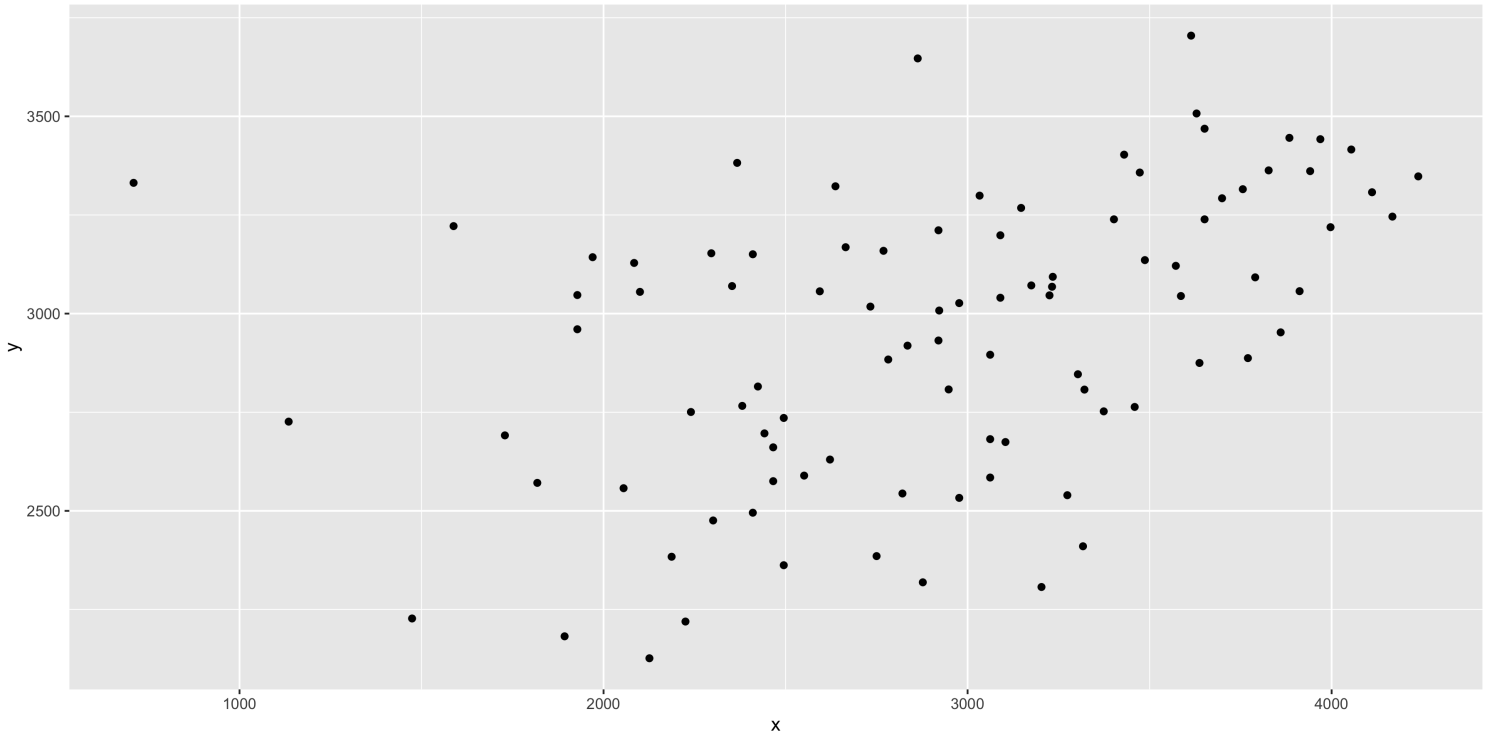
```
odds <- seq(1, nrow(birthwt.noout), by=2)
birthwt.in <- birthwt.noout[odds,]
birthwt.out <- birthwt.noout[-odds,]
linear.model.half <- lm (birthwt.grams ~ . - birthwt.below.2500, data
summary (linear.model.half)
```

```
##
## Call:
## lm(formula = birthwt.grams ~ . - birthwt.below.2500, data = birthwt.in)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1705.17  -303.11    26.48   427.18  1261.57
##
## Coefficients:
##                    Estimate Std. Error t value Pr(>|t|)
## (Intercept)        2514.891    450.245   5.586 2.81e-07 ***
## mother.age            7.052     14.935   0.472  0.63801
## mother.weight         2.683      2.885   0.930  0.35501
## raceother           113.948    224.519   0.508  0.61312
## racewhite           466.219    204.967   2.275  0.02548 *
## mother.smokesYes   -217.218    154.521  -1.406  0.16349
```

```
birthwt.predict <- predict (linear.model.half)
cor (birthwt.in$birthwt.grams, birthwt.predict)
```

```
## [1] 0.508442
```

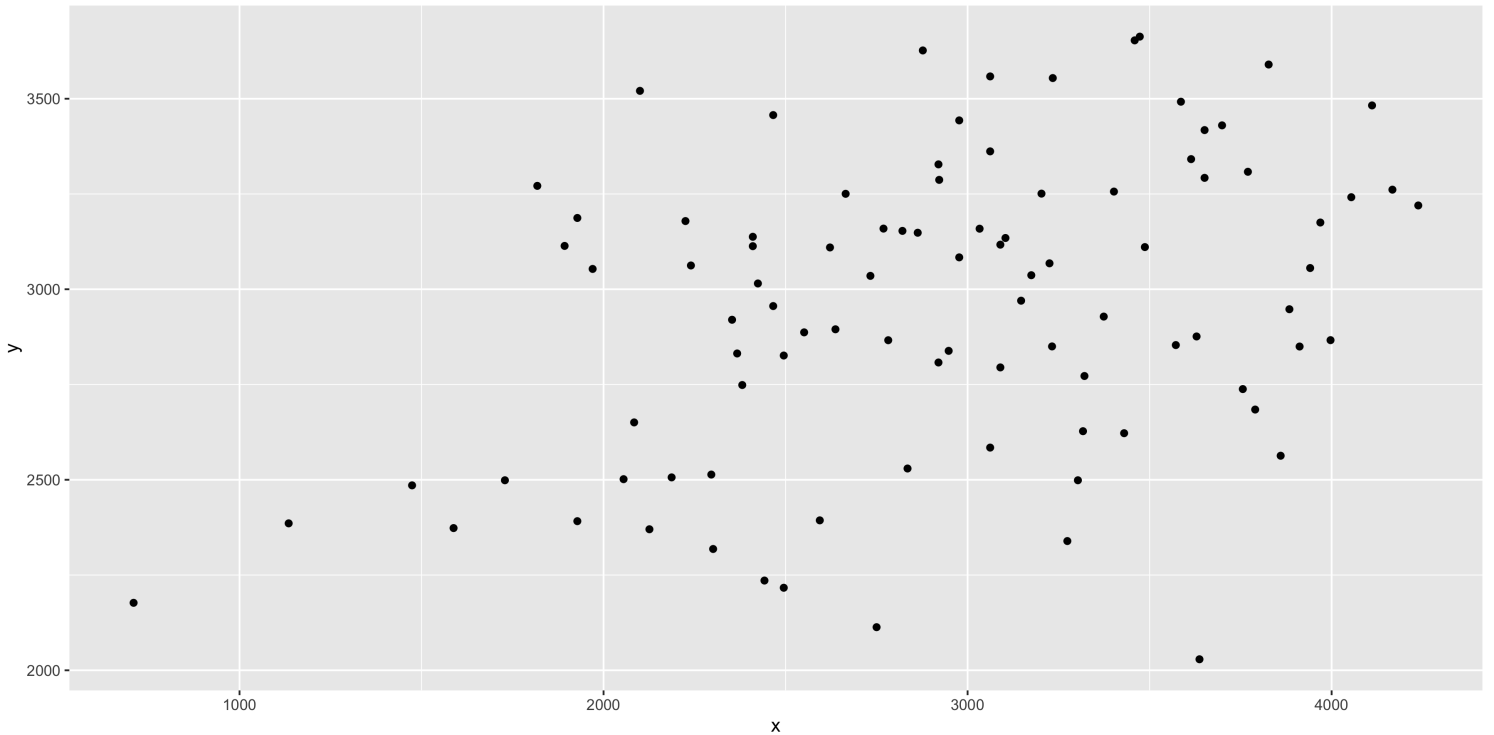
```
tibble(x = birthwt.out$birthwt.grams, y = birthwt.predict) %>%
  ggplot (aes(x = x, y = y)) + geom_point()
```



What Do We Do With This, Anyway?

```
birthwt.predict.out <- predict (linear.model.half, birthwt.out)
cor (birthwt.out$birthwt.grams, birthwt.predict.out)
```

```
## [1] 0.3749431
```



Random number generators

- We made reference to random number generation without going under the hood.
- How *does* R get "random" numbers?
- It doesn't, really -- it uses a trick that should be indistinguishable from the real McCoy

Pseudorandom generators produce a deterministic sequence that is indistiguishable from a true random sequence if you don't know how it started.

Example: `runif`, where we know where it started

```
runif(1:10)
```

```
##  [1] 0.7932482 0.3445822 0.6924252 0.2185041 0.9264878 0.7798071 0.9492686
##  [8] 0.3579187 0.4642079 0.3114528
```

```
set.seed(10)
runif(1:10)
```

```
##  [1] 0.50747820 0.30676851 0.42690767 0.69310208 0.08513597 0.22543662
##  [7] 0.27453052 0.27230507 0.61582931 0.42967153
```

Basic version: Linear Congruential Generator

```
seed <- 10
new.random <- function (a=5, c=12, m=16) {
  out <- (a*seed + c) %% m
  seed <<- out
  return(out)
}
out.length <- 20
variates <- rep (NA, out.length)
for (kk in 1:out.length) variates[kk] <- new.random()
variates
```

```
##  [1] 14  2  6 10 14  2  6 10 14  2  6 10 14  2  6 10 14  2  6 10
```

Try again

Period 8:

```
variates <- rep (NA, out.length)
for (kk in 1:out.length) variates[kk] <- new.random(a=131, c=7, m=16)
variates
```

```
##  [1]  5  6  9  2 13 14  1 10  5  6  9  2 13 14  1 10  5  6  9  2
```

Try again, again

Period 16:

```
variates <- rep (NA, out.length)
for (kk in 1:out.length) variates[kk] <- new.random(a=129, c=7, m=16)
variates
```

```
##  [1]  9  0  7 14  5 12  3 10  1  8 15  6 13  4 11  2  9  0  7 14
```

Try again, at last

Numerical Recipes uses

```
variates <- rep (NA, out.length)
for (kk in 1:out.length) variates[kk] <- new.random(a=1664545, c=1013
variates
```

```
##  [1] 1037207853 2090831916 4106096907  768378826 3835752553 1329121000
##  [7] 2125006663 2668506502 3581687205 2079234980 2067291011 2197025090
## [13] 3748878561 2913996384  758844863 4029469438 2836748829 1458315036
## [19] 2399149563 2766656186
```

How To Distinguish Non-Randomness

- We've covered period: if it's missing some values, it's distinguishable
- Uniformity of distribution in the limitx
- Autocorrelation
- Dimensional distribution -- not a problem for 1-D distributions, but can be for 2+-D

How does R get everything we need?

A few distributions of interest:

- Uniform(0,1)
- Bernoulli(p)
- Binomial(n,p)
- Gaussian(0,1)
- Exponential(1)
- Gamma(a)

In R: everything we need

Suppose we were working with the Exponential distribution.

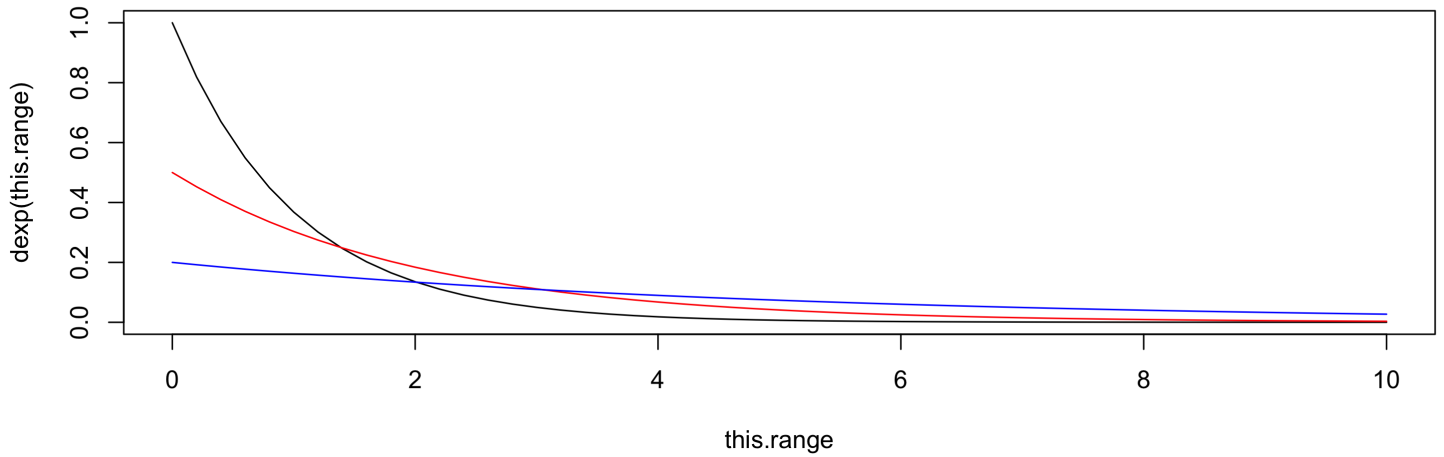
- `rexp()` generates variates from the distribution.
- `dexp()` gives the probability density function.
- `pexp()` gives the cumulative distribution function.
- `qexp()` gives the quantiles.

dexp()

```
dexp(0:5)
```

```
## [1] 1.000000000 0.367879441 0.135335283 0.049787068 0.018315639 0.00673794
```

```
this.range <- 0:50/5
plot (this.range, dexp(this.range), ty="l")
lines (this.range, dexp(this.range, rate=0.5), col="red")
lines (this.range, dexp(this.range, rate=0.2), col="blue")
```

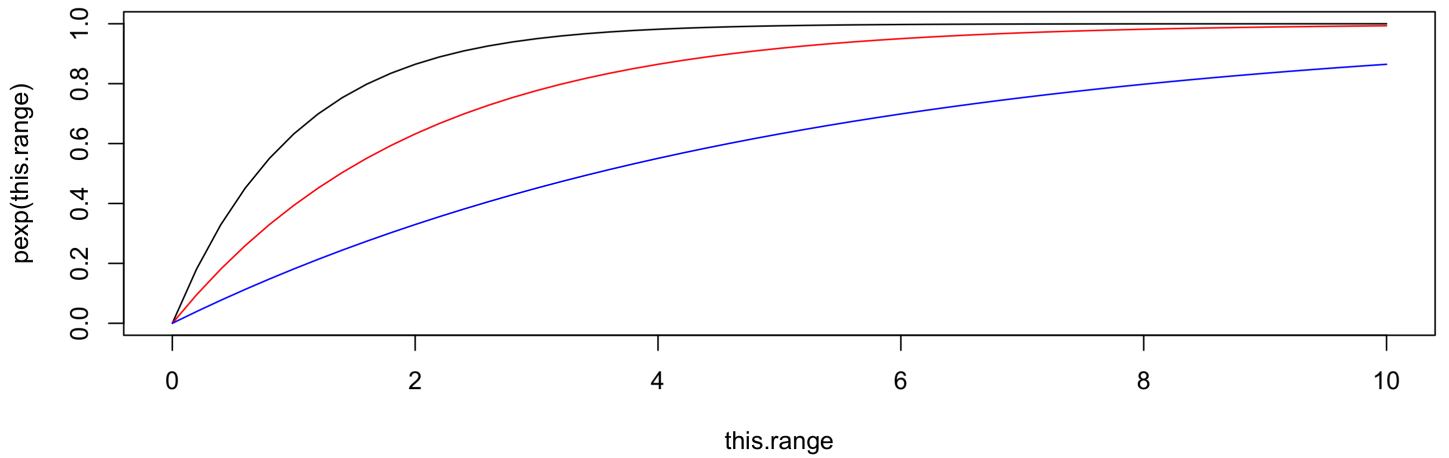


pexp()

```
pexp(0:5)
```

```
## [1] 0.0000000 0.6321206 0.8646647 0.9502129 0.9816844 0.9932621
```

```
this.range <- 0:50/5
plot (this.range, pexp(this.range), ty="l")
lines (this.range, pexp(this.range, rate=0.5), col="red")
lines (this.range, pexp(this.range, rate=0.2), col="blue")
```



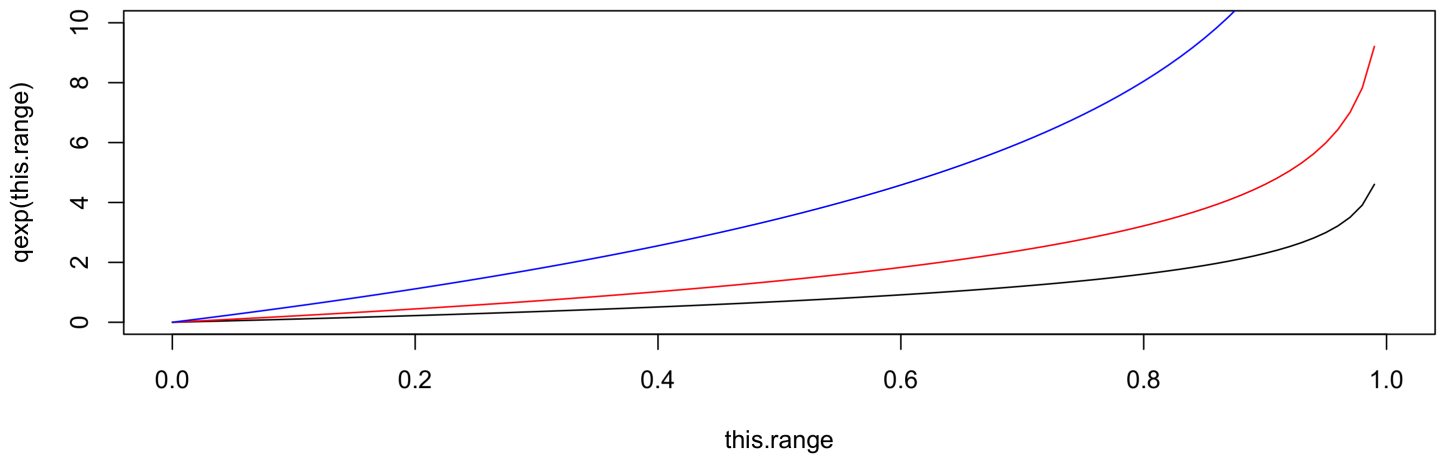
qexp()

```
qexp(0:5)
```

```
## Warning in qexp(0:5): NaNs produced
```

```
## [1]   0 Inf NaN NaN NaN NaN
```

```
this.range <- seq(0,1,by=0.01)
plot (this.range, qexp(this.range), ylim = c(0, 10), ty="l")
lines (this.range, qexp(this.range, rate=0.5), col="red")
lines (this.range, qexp(this.range, rate=0.2), col="blue")
```

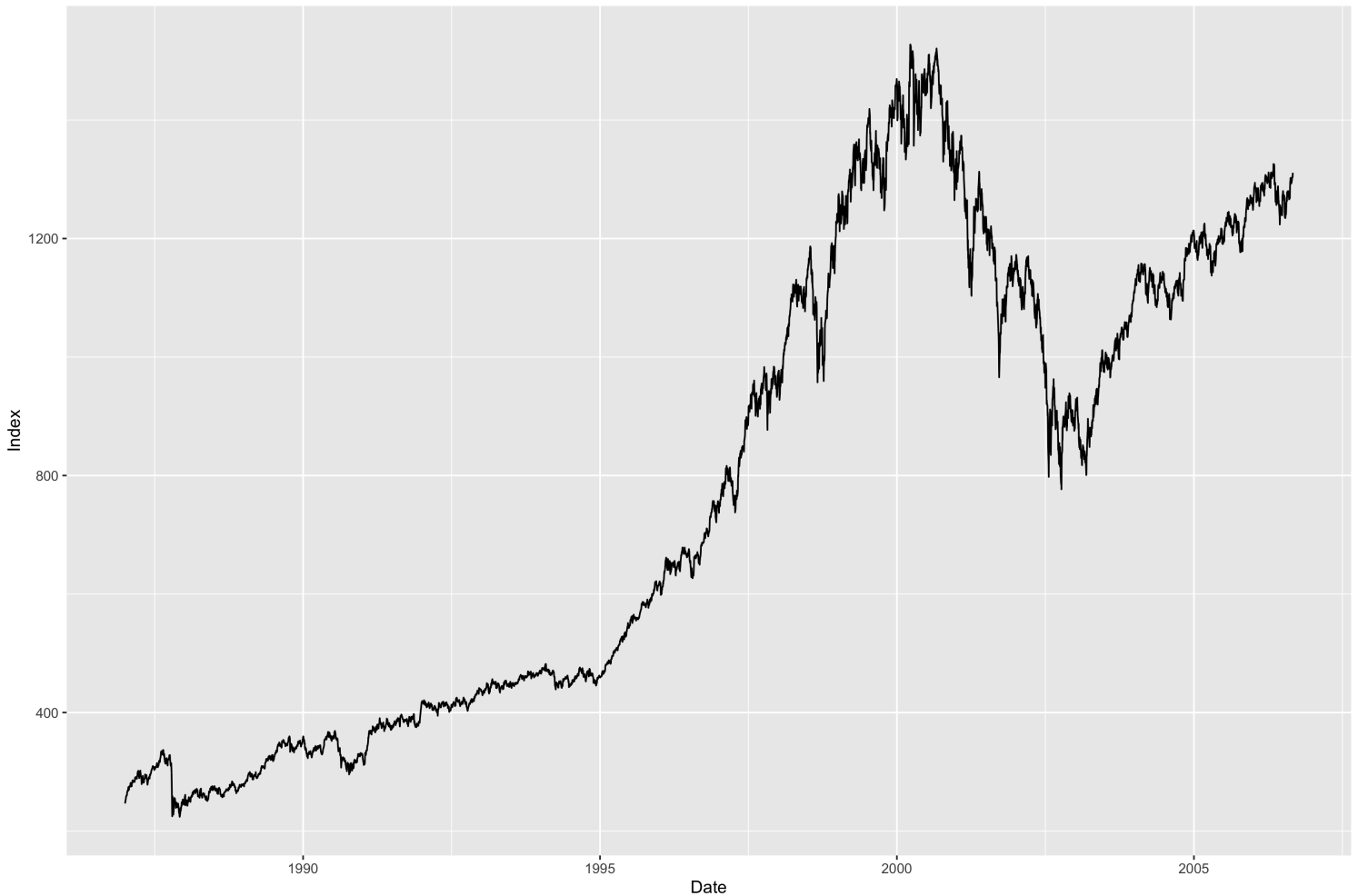


Let's Grab some Data

The Standard and Poor's 500, or simply the S\&P 500, is a stock market index tracking the stock performance of 500 large companies listed on exchanges in the United States. It is one of the most commonly followed equity indices.

```
library(readxl)
SP <- read_excel("data/Stock_Bond.xls") %>% dplyr::select(Date, `S&P_
  rename(Index = `S&P_AC`)
```

```
SP %>% ggplot(aes(x = Date, y = Index)) + geom_line()
```



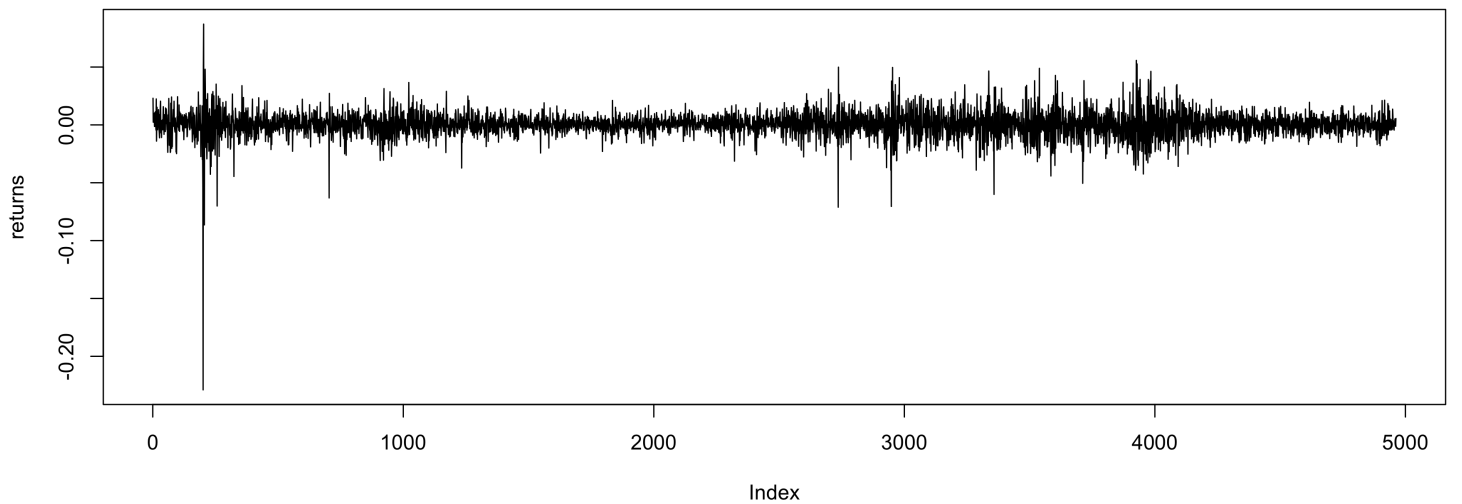
Let's Transform Some Data

The price p_t doesn't matter, what matters are the returns $r_t = \log(p_t/p_{t-1})$

```
returns <- na.omit(as.vector(diff(log(SP$Index))))
summary(returns)
```

```
##        Min.    1st Qu.     Median       Mean    3rd Qu.       Max.
## -0.2289972 -0.0046537  0.0004976  0.0003368  0.0056195  0.0870888
```

```
plot(returns, type="l")
```



The Data's Distribution

`quantile(x,probs)` calculates the quantiles at `probs` from `x`

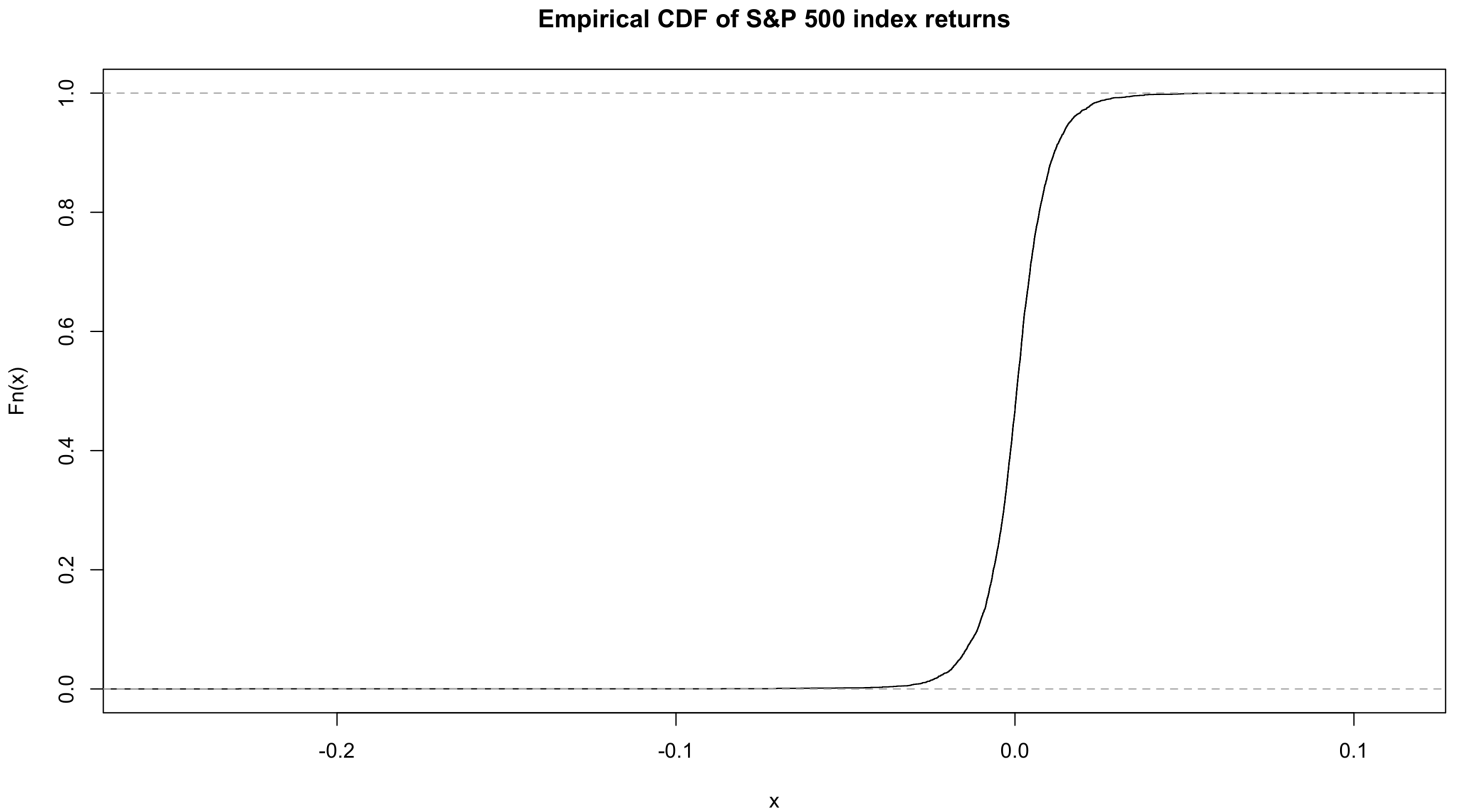
```
quantile(returns,c(0.25,0.5,0.75))
```

```
##            25%            50%            75%
## -0.0046537538  0.0004976042  0.0056195438
```

`ecdf()` - *e* mpirical *c* umulative *d* istribution *f* unction; no assumptions but also no guess about distribution between the observations

In math, ECDF is often written as $\hat{F}$ or $\hat{F}_n$

```
plot(ecdf(returns), main="Empirical CDF of S&P 500 index returns")
```



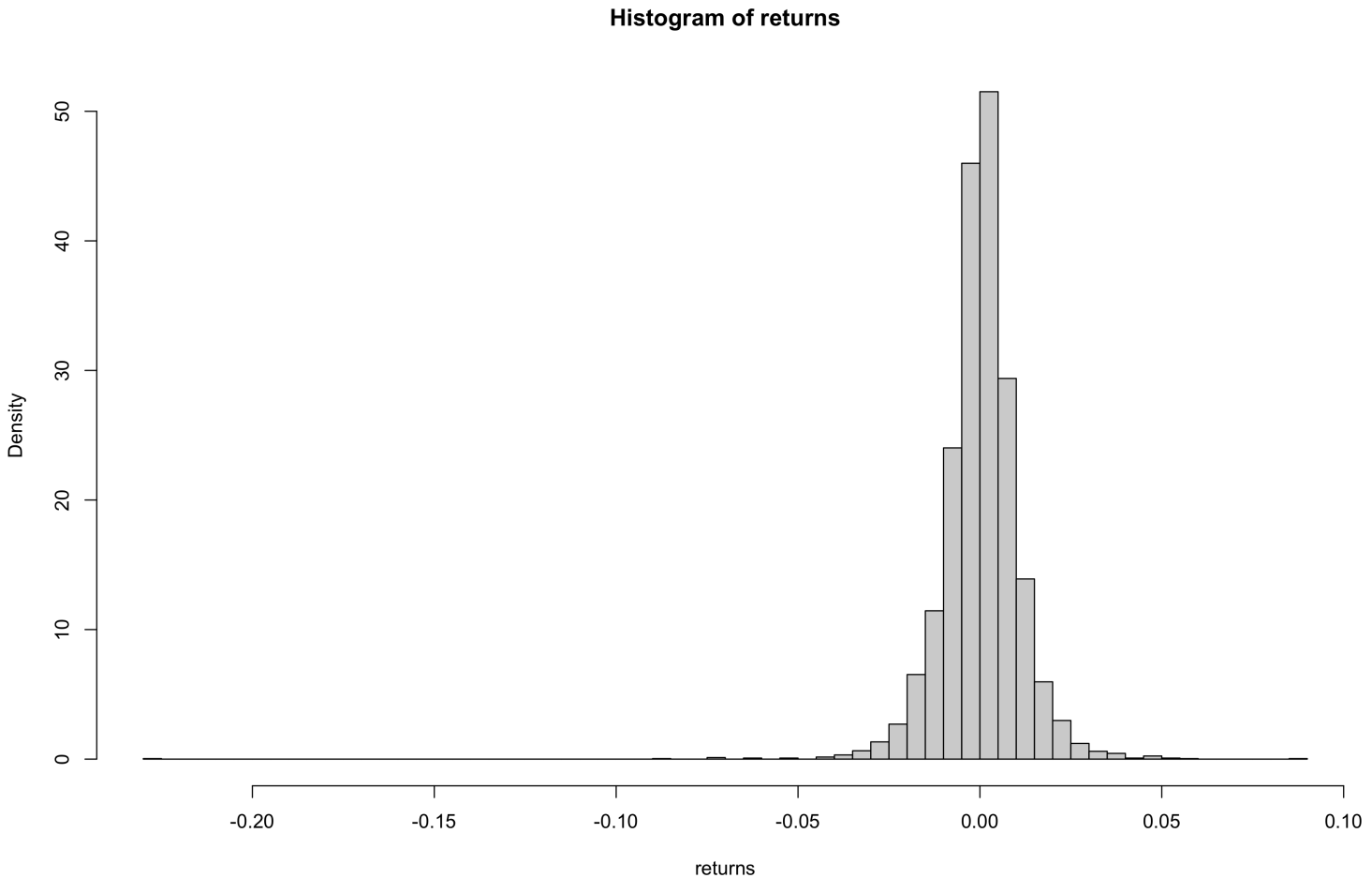
Conceptually, `quantile` and `ecdf` are inverses to each other

Getting Probability Densities from Data

`hist(x)` calculates a histogram from `x`

- divide the data range up into equal-width bins and *count* how many fall into each bin
- *Or* divide bin counts by (total count)*(width of bin), and get an estimate of the probability density function (pdf)
  Produces plot as a default side-effect

```
hist(returns,n=101,probability=TRUE)
```



Probability Densities from Data (cont'd.)

`density(x)` estimates the density of `x` by counting how many observations fall in a little window around each point, and then smoothing

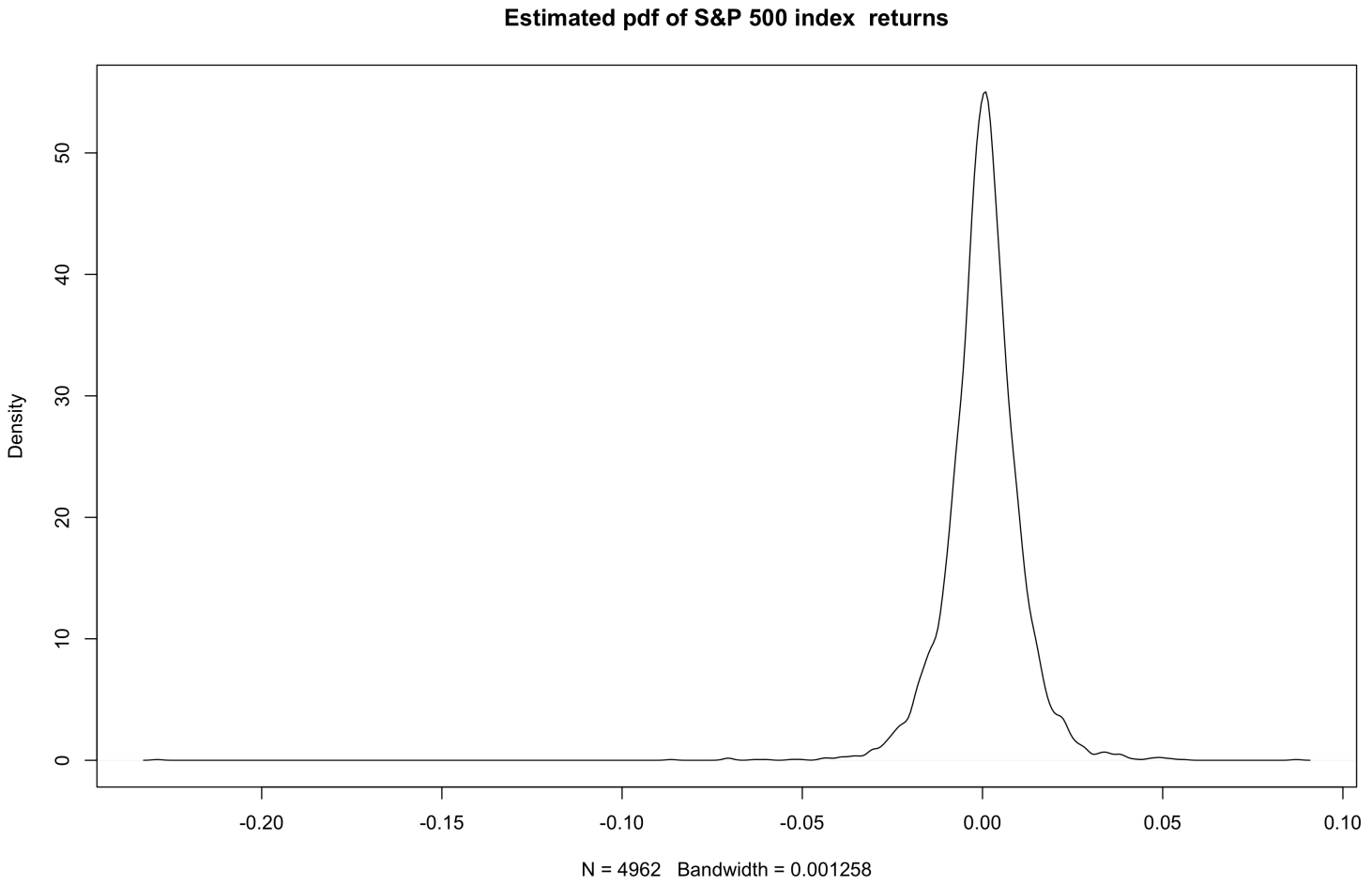
"Bandwidth" $\approx$ width of window around each point

Technically, a "kernel density estimate"

Remember: `density()` is an *estimate* of the pdf, not The Truth

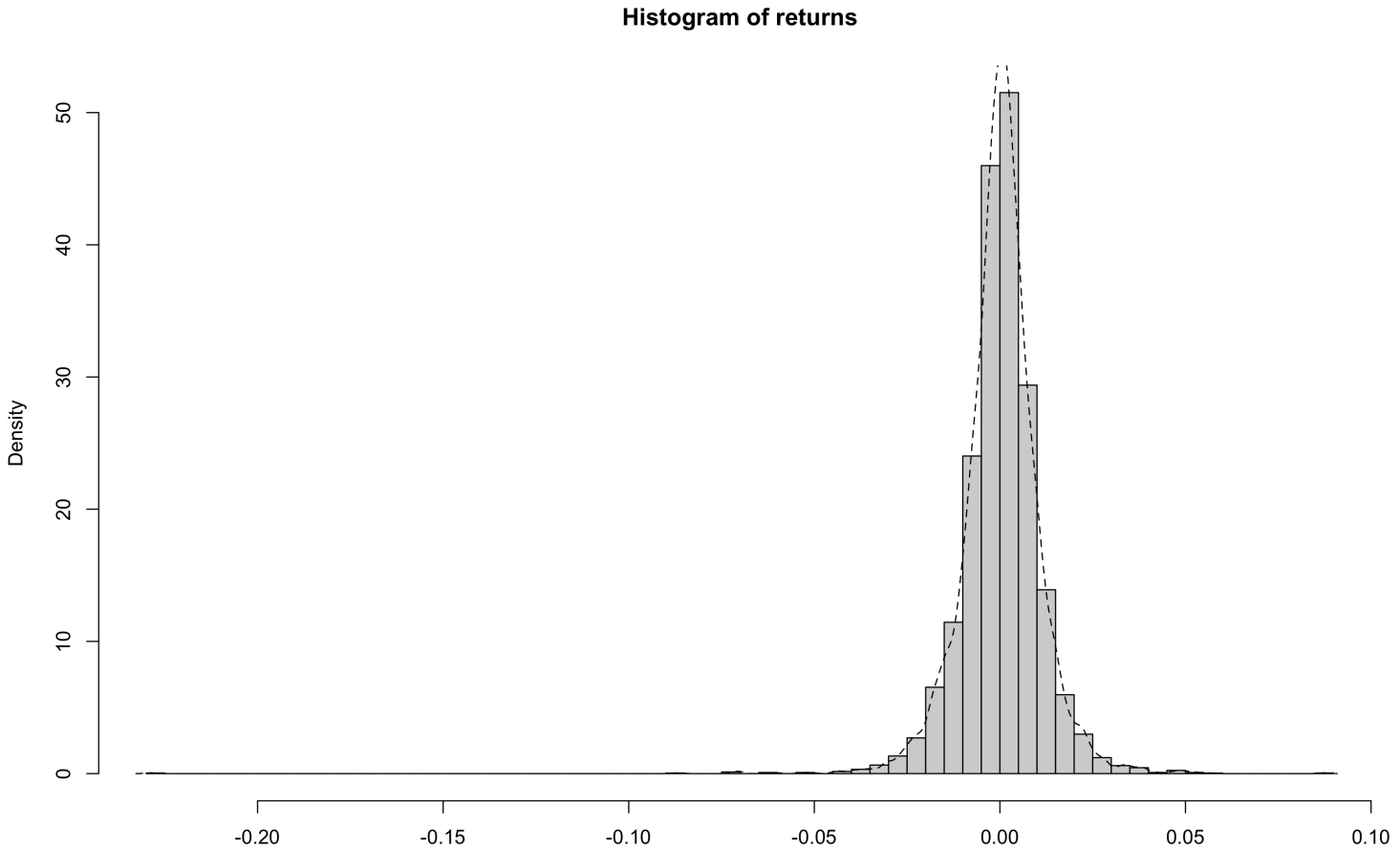
`density` returns a collection of x, y values, suitable for plotting

```
plot(density(returns),main="Estimated pdf of S&P 500 index  returns")
```



Probability Densities from Data (cont'd.)

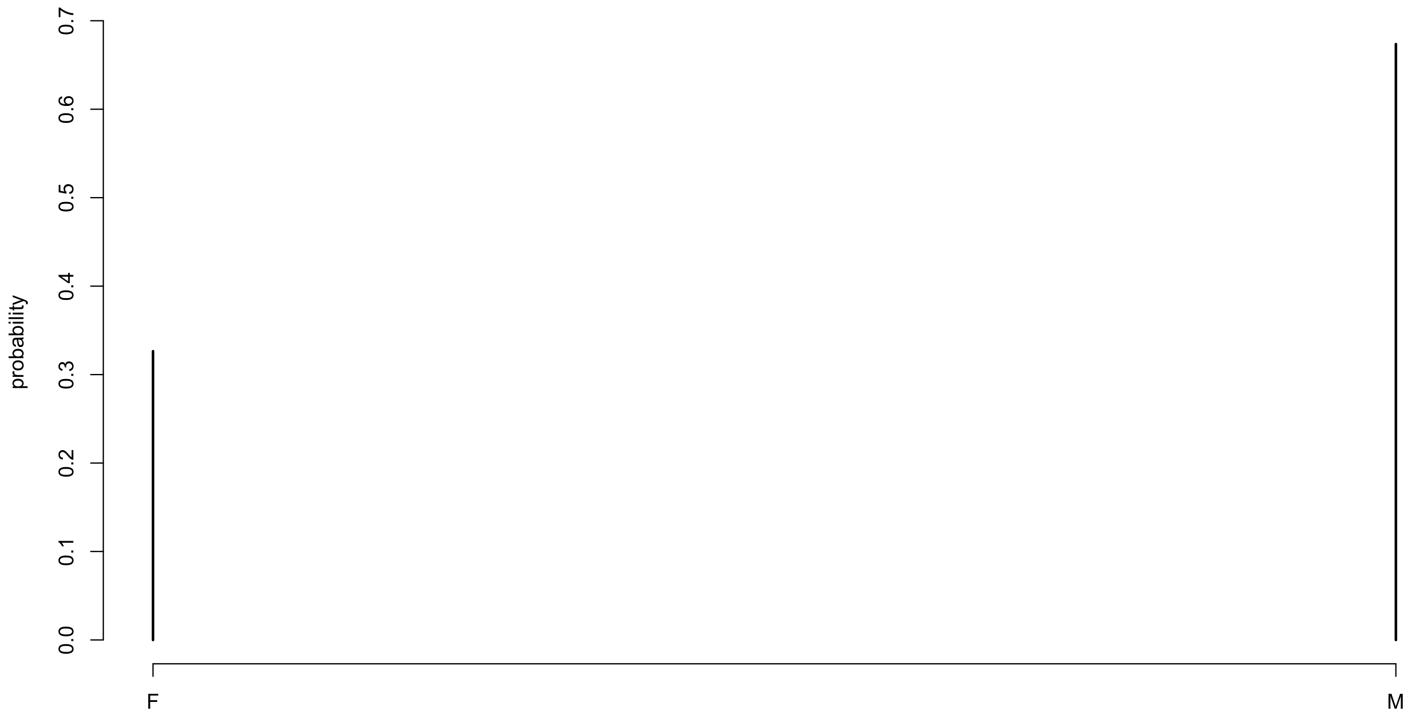
```
hist(returns,n=101,probability=TRUE)
lines(density(returns),lty="dashed")
```



Getting distributions from data (cont'd.)

`table()` - tabulate outcomes, most useful for discrete spaces; remember to normalize if you want probabilities

```
plot(table(cats$Sex)/nrow(cats),ylab="probability")
```



Who Cares About the Distribution of the Data?

- Overly detailed: every single observation recorded as a separate tick
  - *Too much information*
- The exact set of samples would never repeat if we re-ran things anyway
  - *That information is wrong*
- Try to *summarize* what will *generalize* to other situations
  - Use a model, remember the model's parameters

R commands for distributions

- d*foo* = the probability *d* ensity (if continuous) or probability mass function of *foo* (pdf or pmf)
- p*foo* = the cumulative *p* robability function (CDF)
- q*foo* = the *q* uantile function (inverse to CDF)
- `r`*foo* = draw *r* andom numbers from `foo` (first argument always the number of draws)

`?Distributions` to see which distributions are built in

If you write your own, follow the conventions

Examples

```
dnorm(x=c(-1,0,1),mean=1,sd=0.1)
```

```
## [1] 5.520948e-87 7.694599e-22 3.989423e+00
```

```
pnorm(q=c(2,-2)) # defaults to mean=0,sd=1
```

```
## [1] 0.97724987 0.02275013
```

```
dbinom(5,size=7,p=0.7,log=TRUE)
```

```
## [1] -1.146798
```

```
qchisq(p=0.95,df=5)
```

```
## [1] 11.0705
```

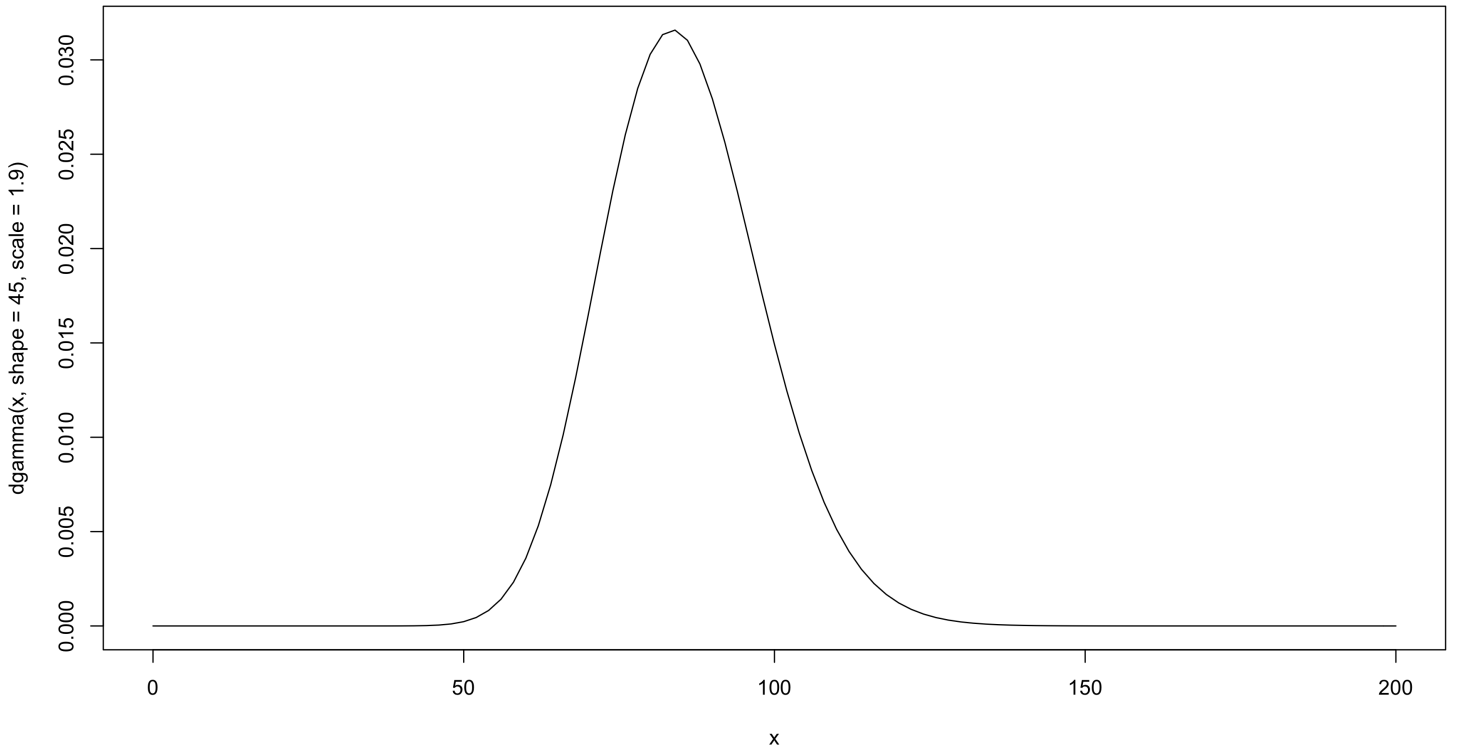
```
rt(n=4,df=2)
```

```
## [1]  0.4397369  1.1463390 -0.3783058 -1.3546069
```

Displaying Probability Distributions

`curve` is very useful for the `d`, `p`, `q` functions:

```
curve(dgamma(x,shape=45,scale=1.9),from=0,to=200)
```



How Do We Fit Distributional Models to the Data?

- Match moments (mean, variance, etc.)
- Match other summary statistics
- Maximize the likelihood

Method of Moments (MM), Closed Form

- Pick enough moments that they **identify** the parameters
  - At least 1 moment per parameter; algebraically independent
- Write equations for the moments in terms of the parameters
  e.g., for gamma

$$\mu = as \ , \ \sigma^2 = as^2$$

- Do the algebra by hand to solve the equations

$$a = \mu^2/\sigma^2 \ , \ s = \sigma^2/\mu$$

- Code up the formulas (did this in lab 3)

```
gamma.est_MM <- function(x) {
  m <- mean(x); v <- var(x)
  return(c(shape=m^2/v, scale=v/m))
}
```

MM, Numerically

- Write functions to get moments from parameters (usually algebra)
- Set up the difference between data and model as another function

```
gamma.mean <- function(shape,scale) { return(shape*scale) }
gamma.var <- function(shape,scale) { return(shape*scale^2) }
gamma.discrepancy <- function(shape,scale,x) {
  return((mean(x)-gamma.mean(shape,scale))^2 + (var(x)-gamma.mean(shape,scale
}
```

- Minimize it

More Generally...

- Nothing magic about moments
- Match other data summaries, say the median
  - Or even more complicated things, like ratios of quantiles
  - You did this in lab
- If you can't solve exactly for parameters from the summaries, set up a discrepancy function and minimize it
  - You are doing this in the HW
- The summaries just have to converge on population values

Maximum Likeihood

- Usually we think of the parameters as fixed and consider the probability of different outcomes, $f(x;\theta)$ with θ constant and x changing
- **Likelihood** of a parameter value = $L(\theta)$ = what probability does θ give to the data?
  - For continuous variables, use probability density
  - $f(x;\theta)$ but letting θ change while data constant
  - *Not* the probability of θ, if that even makes sense
- **Maximum likelihood** = guess that the parameter is whatever makes the data most likely
- Most likely parameter value = **maximum likelihood estimate** = **MLE**

Likelihood in Code

- With independent data points x_1, x_2, x_n, likelihood is

$$L(\theta) = \prod_{i=1}^{n} f(x_i; \theta)$$

- Multiplying lots of small numbers is numerically bad; take the log:

$$\ell(\theta) = \sum_{i=1}^{n} \log f(x_i; \theta)$$

- In pseudo-code:

```
loglike.foo <- function(params, x) {
  sum(dfoo(x=x,params,log=TRUE))
}
```

What Do We Do with the Likelihood?

- We maximize it!
- Sometimes we can do the maximization by hand with some calculus
  - For Gaussian, MLE = just match the mean and variance
  - For Pareto, MLE $\widehat{a} = 1 + 1/\overline{\log\left(x/x_{\min}\right)}$
- Doing numerical optimization
  - Stick in a minus sign if we're using a minimization function

Why Use the MLE?

- Usually (but not always) *consistent*: converges on the truth as we get more data
- Usually (but not always) *efficient*: converges on the truth at least as fast as anything else
- There are some parameters where the maximum isn't well-defined (e.g. $x_{\min}$ for a Pareto)
- Sometimes the data is too aggregated or mangled to use the MLE (as with the income data in lab 5)

fitdistr

MLE for one-dimensional distributions can be done through `fitdistr` in the `MASS` package

It knows about most the standard distributions, but you can also give it arbitrary probability density functions and it will try to maximize them
A starting value for the optimization is optional for some distributions, required for others (including user-defined densities)

Returns the parameter estimates and standard errors
SEs come from large n approximations so use cautiously

fitdistr Examples

Fit the gamma distribution to the cats' hearts:

```
require(MASS)
fitdistr(cats$Hwt, densfun="gamma")
```

```
##      shape          rate
##   20.2998092    1.9095724
##  ( 2.3729243) ( 0.2259941)
```

Returns: estimates above, standard errors below

Fit the Students t distribution to the returns:

```
fitdistr(returns,"t")
```

```
##          m                s               df
##   0.0005103602   0.0071003759   3.5882142132
##  (0.0001206711) (0.0001290377) (0.2076615056)
```

Here parameters are location (m), scale (s) and degrees of freedom (very heavy tails)

fitdistr Examples (cont'd.)

User-defined density:

```
dpareto <- function(x,exponent,xmin,log=FALSE) {
  f <- (exponent-1)/xmin * (x/xmin)^(-exponent)
  f <- ifelse(x<xmin,NA,f)
  if(!log) { return(f) } else (return(log(f)))
}
# Fit pareto to large absolute returns
  # Parameters given outside the "start" list are fixed
fitdistr(abs(returns)[abs(returns)>0.05], densfun=dpareto,
         start=list(exponent=2.5), xmin=0.05)
```

```
## Warning in stats::optim(x = c(0.0529756421537337, 0.228997226565671, 0.051
## use "Brent" or optimize() directly

##    exponent
##   3.9960938
##  (0.8309668)
```

Checking Your Estimator

- simulate, then estimate; estimates should converge as the sample grows

```
gamma.est_MM(rgamma(100,shape=19,scale=45))
```

```
##    shape    scale
## 20.72856 41.69062
```

```
gamma.est_MM(rgamma(1e5,shape=19,scale=45))
```

```
##    shape    scale
## 19.00673 44.88559
```

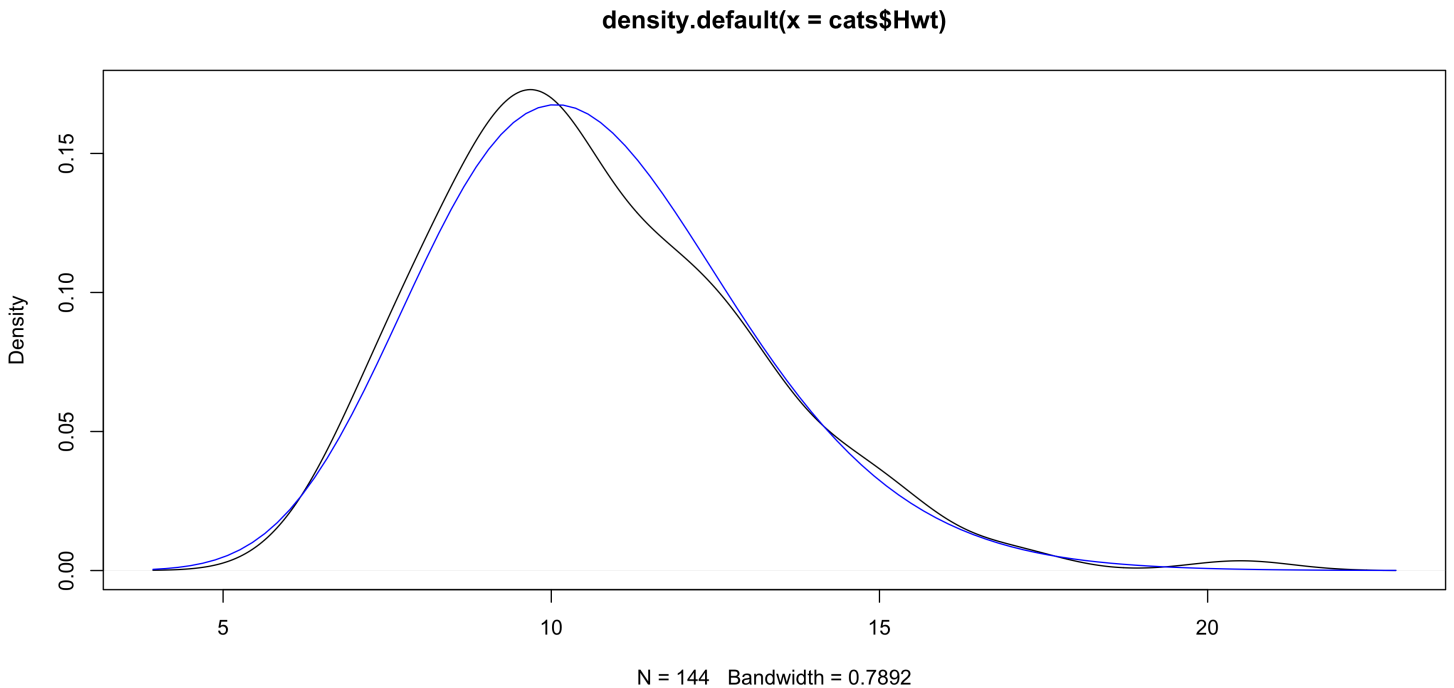
```
gamma.est_MM(rgamma(1e6,shape=19,scale=45))
```

```
##    shape    scale
## 18.99762 45.01647
```

Checking the Fit

Use your eyes: Graphic overlays of theory vs. data

```
plot(density(cats$Hwt))
cats.gamma <- gamma.est_MM(cats$Hwt)
curve(dgamma(x,shape=cats.gamma["shape"],scale=cats.gamma["scale"]),a
```



Checking the Fit (cont'd.)

- Calculate summary statistics *not* used in fitting, compare them to the fitted model

```
# Really bad and good days for index fund holders, per model:
qnorm(c(0.01,0.99),mean=mean(returns),sd=sd(returns))
```

```
## [1] -0.02487668  0.02555036
```

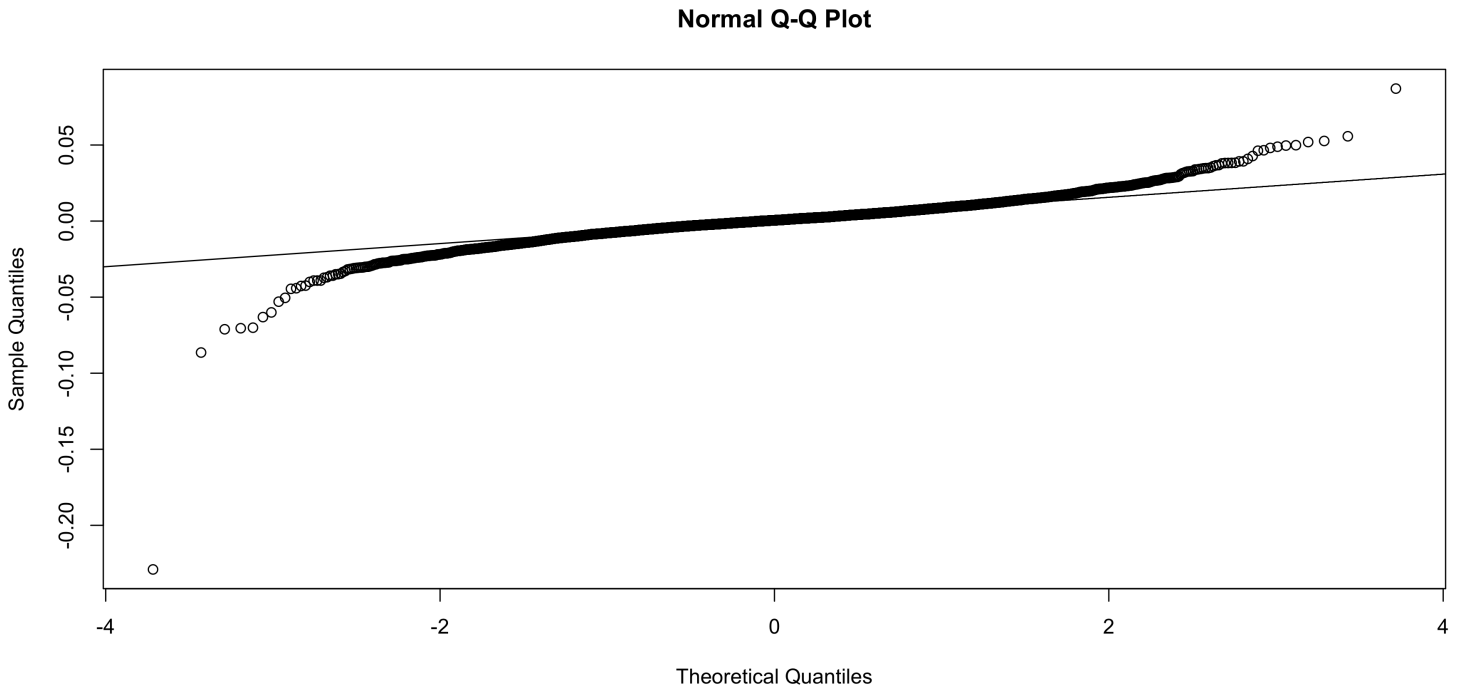
```
# As it happened:
quantile(returns,c(0.01,0.99))
```

```
##           1%          99%
## -0.02730130  0.02765495
```

Quantile-Quantile (QQ) Plots

- Plot theoretical vs. actual quantiles
- *or* plot quantiles of two samples against each other
- Ideally, a straight line when the distributions are the same
- `qqnorm`, `qqline` are specialized for checking normality

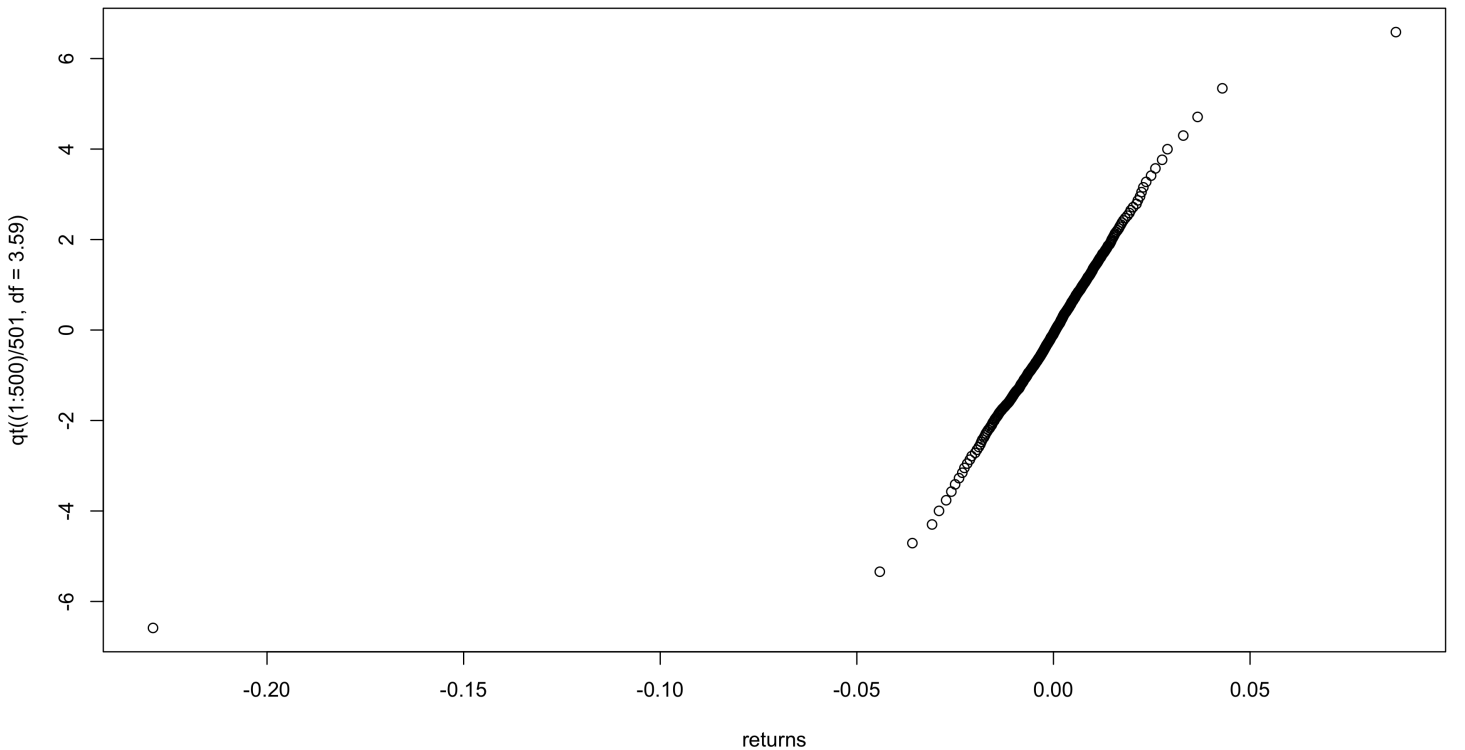
```
qqnorm(returns); qqline(returns)
```



QQ Plots (cont'd)

- `qqplot(x,y)` will do a Q-Q plot of one vector against another

```
qqplot(returns,qt((1:500)/501,df=3.59))
```

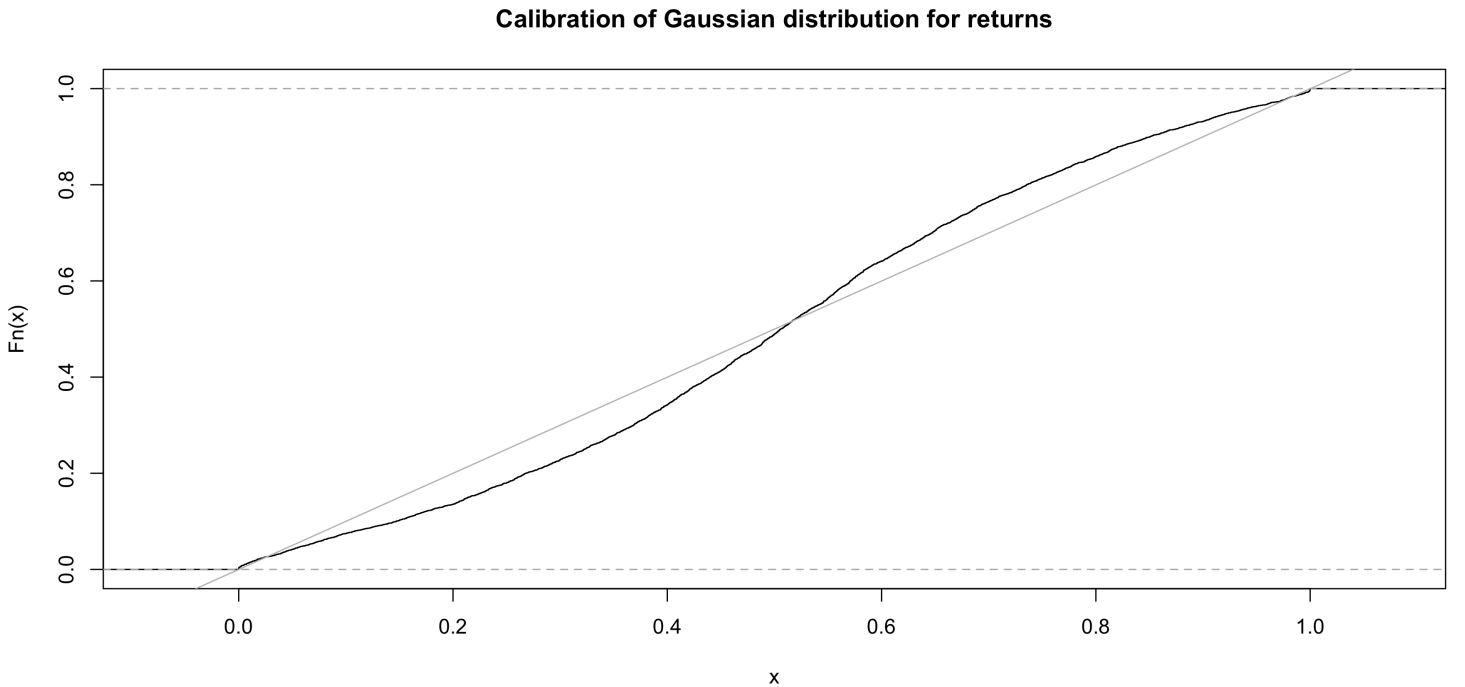


Calibration Plots

- If the distribution is right, 50% of the data should be below the median, 90% should be below the 90th percentile, etc.
- Special case of **calibration** of probabilities: events with probability p% should happen about p% of the time, not more and not less
- We can look at calibraton by calculating the (empirical) CDF of the (theoretical) CDF and plotting
  - Ideal calibration plot is a straight line up the diagonal
  - Systematic deviations are a warning sign

Making a Calibration Plot

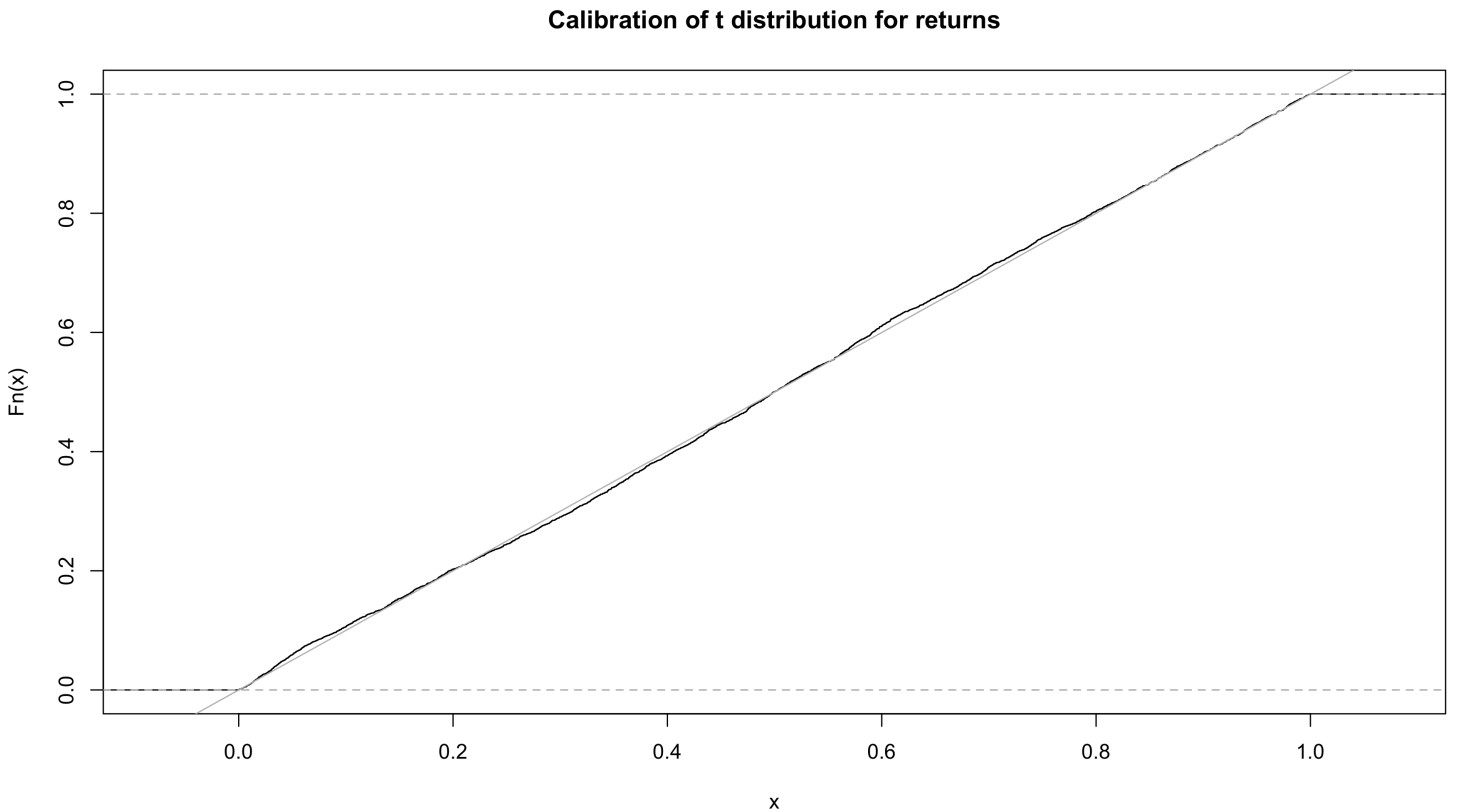
```
plot(ecdf(pnorm(returns, mean=mean(returns), sd=sd(returns))),
     main="Calibration of Gaussian distribution for returns")
abline(0,1,col="grey")
```



Again, way too many large changes (in either direction)

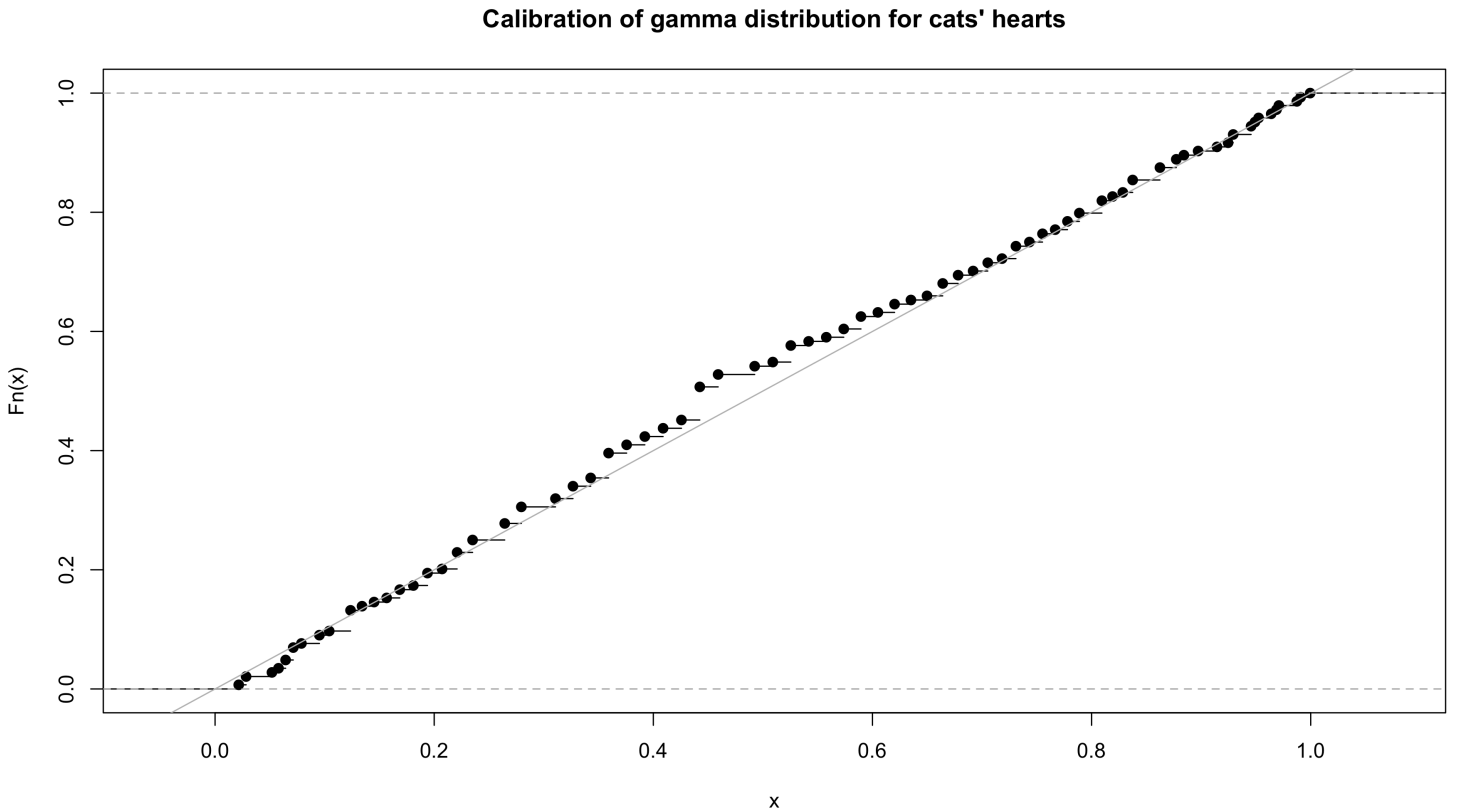
Calibration Plots (cont'd.)

```
SP.t <- coefficients(fitdistr(returns,"t"))
plot(ecdf(pt((returns-SP.t[1])/SP.t[2], df=SP.t[3])),
     main="Calibration of t distribution for returns")
abline(0,1,col="grey")
```



Calibration Plots (cont'd.)

```
plot(ecdf(pgamma(cats$Hwt, shape=cats.gamma["shape"], scale=cats.gamm
     main="Calibration of gamma distribution for cats' hearts")
abline(0,1,col="grey")
```



Calibration Plots (cont'd.)

Challenge: Write a general function for making a calibraton plot, taking a data vector, a cumulative probability function, and a parameter vector

Kolmogorov-Smirnov Test

- How much should the QQ plot or calibration plot wiggle around the diagonal?
- Answer a different question…
- Biggest gap between theoretical and empirical CDF:

$$D_{KS} = \max_x \left| F(x) - \widehat{F}(x) \right|$$

- Useful because D_{KS} always has the same distribution *if* the theoretical CDF is fixed and correct, and K+S calculated this back in the day
- Also works for comparing the empirical CDFs of two samples, to see if they came from the same distribution

KS Test, Data vs. Theory

```
ks.test(returns,pnorm,mean=0,sd=0.0125)
```

```
##
##     One-sample Kolmogorov-Smirnov test
##
## data:  returns
## D = 0.10893, p-value < 2.2e-16
## alternative hypothesis: two-sided
```

- More complicated (and *not* properly handled by built-in R) if parameters are estimated
  - Estimating parameters makes the fit look *better* than it really is, so it doesn't help save the model when it gets really rejected (like this one is)

Hack: Estimate using (say) 90% of the data, and then check the fit on the remaining 10%

```
train <- sample(1:length(returns),size=round(0.9*length(returns)))
SP.t_train <- coefficients(fitdistr(returns[train],"t"))
returns.test_standardized <- (returns[-train]-SP.t_train[1])/SP.t_tra
ks.test(returns.test_standardized,pt,df=SP.t_train[3])
```

```
##
##     One-sample Kolmogorov-Smirnov test
##
## data:  returns.test_standardized
## D = 0.037817, p-value = 0.4772
## alternative hypothesis: two-sided
```

- Can also test whether two samples come from same distribution

```
n <- length(returns)
half <- round(n/2)
ks.test(returns[1:half], returns[(half+1):n])
```

```
##
##     Two-sample Kolmogorov-Smirnov test
##
## data:  returns[1:half] and returns[(half + 1):n]
## D = 0.099154, p-value = 5.103e-11
## alternative hypothesis: two-sided
```

Chi-Squared Test for Discrete Distributions

Compare an actual table of counts to a hypothesized probability distribution

e.g., as many up days as down?

```
up_or_down <- ifelse(returns > 0, 1, -1)
# 1936 down days, 1772 up days
chisq.test(table(up_or_down),p=c(1/2,1/2))
```

```
##
##     Chi-squared test for given probabilities
##
## data:  table(up_or_down)
## X-squared = 20.896, df = 1, p-value = 4.85e-06
```

Chi-Squared Test: Degrees of Freedom

- The p-value calculated by `chisq.test` assumes that all the probabilities in p were *fixed*, not estimated from the data used for testing, so `df` = number of cells in the table -1
- If we estimate q parameters, we need to subtract q degrees of freedom

Chi-Squared Test for Continuous Distributions

- Divide the range into bins and count the number of observations in each bin; this will be `x` in `chisq.test()`
- Use the CDF function `p`*foo* to calculate the theoretical probability of each bin; this is `p`
- Plug in to `chisq.test`

- If parameters are estimated, adjust

- `hist()` gives us break points and counts:

```
cats.hist <- hist(cats$Hwt,plot=FALSE)
cats.hist$breaks
```

```
## [1]  6  8 10 12 14 16 18 20 22
```

```
cats.hist$counts
```

```
## [1] 20 45 42 23 11  2  0  1
```

Chi-Squared for Continuous Data (cont'd.)

Use these for a χ^2 test:

```
# Why the padding by -Inf and Inf?
p <- diff(pgamma(c(-Inf,cats.hist$breaks,Inf),shape=cats.gamma["shape
                 scale=cats.gamma["scale"]))
# Why the padding by 0 and 0?
x2 <- chisq.test(c(0,cats.hist$counts,0),p=p)$statistic
# Why +2? Why -length(cats.gamma)?
pchisq(x2,df=length(cats.hist$counts)+2 - length(cats.gamma))
```

```
## X-squared
##  0.854616
```

Don't need to run `hist` first; can also use `cut` to discretize (see `?cut`)

- This is all a bit old-school
  - Loss of information from discretization
  - Lots of work just to use χ^2
- Try e.g. `ks.test` with an independent test set

Summary

- Visualizing and computing empirical distribution
- Parametric distributions are models
- Methods of fitting: moments, generalized moments, likelihood
- Methods of checking: visual comparisons, other statistics, tests, calibration

Aside: Some Math for MM and GMM

- Parameter θ is a p-dimensional vector, true value = θ^*
- Introduce $q \geq p$ **functionals** $g_1, \ldots g_q$, which we can calculate either from the parameter θ or from the data $x_{1:n}$
- *Assume* that for each i, $g_i(x_{1:n}) \to g_i(\theta^*)$
- *Define*

$$\hat{\theta}_{GMM} = \text{argmin}_\theta \sum_{i=1}^{q} (g_i(\theta) - g_i(x_{1:n}))^2$$

Math for MM and GMM (cont'd.)

- Shouldn't be hard to believe that $\hat{\theta}_{GMM} \to \theta^*$
- But why give equal attention to every functional?
  - More weight on the more-precisely-measured functionals
  - More weight on the more-sensitive-to θ functionals
  - Less weight on partially-redundant functionals
- *Abbreviate* $g(\theta)$ for $(g_1(\theta), \ldots g_q(\theta))$, and likewise $g(x_{1:n})$, so

$$\hat{\theta}_{GMM} = \text{argmin}_\theta (g(\theta) - g(x_{1:n}))^T (g(\theta) - g(x_{1:n}))$$

- Generalize by introducing any positive-definite matrix Ω:

$$\hat{\theta}_{GMM} = \text{argmin}_\theta (g(\theta) - g(x_{1:n}))^T \Omega (g(\theta) - g(x_{1:n}))$$

- Optimal Ω turns out to be the variance matrix of $g(\theta^*)$
- Iterative approximation: start with no weighting, estimate that variance matrix, re-do the estimate with weights, etc.

Aside: Some Math for the MLE

- More convenient to work with the mean log likelihood:

$$\Lambda(\theta) = \frac{1}{n}\sum_{i=1}^{n} \log f(X_i; \theta)$$

- This is a sample average so the law of large numbers applies:

$$\Lambda(\theta) \to \mathbf{E}[\Lambda(\theta)] = \lambda(\theta)$$

- The true parameter has higher average log-likelihood than anything else: if $\theta \neq \theta^*$

$$\theta \neq \theta^* \;\Rightarrow \lambda(\theta) < \lambda(\theta^*)$$

- Some extra conditions are needed for

$$\hat{\theta}_{MLE} \to \theta^*$$