STAT 513/413: Lecture 11
Sampling and resampling

(bootstrap, permutation tests, and all that)

What we cannot establish by probabilistic calculations, we accomplish by simulations

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Rizzo 7.1, 7.2, 7.3, 8.1

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The median: recall

The *median* of a probability distribution P is defined to be a number m such that

$$P((-\infty, m]) \geqslant 1/2 \qquad \text{and} \qquad P[(m, +\infty)) \geqslant 1/2$$

A very common situation is that

$$P((-\infty, m] = P[(m, +\infty)) = 1/2$$

In such a case, the median is $Q(0.5) = F^{-1}(0.5)$

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where F is the cumulative distribution function of P

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Right now, we are not interested in what is the median, μ, of the distribution, but we are interested its estimator M_{10}, the *sample median*, taken out of sample of 10 numbers that look like the outcomes of independent random variables with exponential distribution with $\lambda = 1$: how does it perform?

For starters: one of the performance measures of an estimator is its variance

Variance is easy: but is it the right thing here?

```
> var(replicate(100,median(rexp(10))))
[1] 0.09402476
> var(replicate(100,median(rexp(10))))
[1] 0.09007331
> var(replicate(100,median(rexp(10))))
[1] 0.08155923
> var(replicate(1000,median(rexp(10))))
[1] 0.09270415
> var(replicate(1000,median(rexp(10))))
[1] 0.09723465
> var(replicate(1000,median(rexp(10))))
[1] 0.09982106
> var(replicate(100000,median(rexp(10))))
[1] 0.09628878
> var(replicate(100000,median(rexp(10))))
[1] 0.09590175
```

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Note the difference: M_{10} estimates m out of $n = 10$ numbers

while T_N estimates Var(M_{10}) out of $N = 100000$ results

Is M_{10} an unbiased estimator of m?

A general measure of the quality of the estimator is the mean squared error $\mathsf{E}\left[(M_{10} - m)^2\right]$. The variance is linked to it through bias-variance decomposition

$$
\begin{aligned}
\mathsf{E}\left[(M_{10} - m)^2\right] &= \mathsf{E}\left[(M_{10} - \mathsf{E}(M_{10}))^2\right] + \mathsf{E}\left[(\mathsf{E}(M_{10}) - m)^2\right] \\
&\quad + \mathsf{E}\left[2(M_{10} - \mathsf{E}(M_{10}))(\mathsf{E}(M_{10}) - m)\right] \\
&= \mathsf{Var}(M_{10}) + (m - \mathsf{E}(M_{10}))^2
\end{aligned}
$$

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as

$$
\begin{aligned}
\mathsf{E}\left[2(M_{10} - \mathsf{E}(M_{10}))(\mathsf{E}(M_{10}) - m)\right] &= 2(\mathsf{E}(M_{10}) - m)\,\mathsf{E}\left[M_{10} - \mathsf{E}(M_{10})\right] \\
&= 2(\mathsf{E}(M_{10}) - m)(\mathsf{E}(M_{10}) - \mathsf{E}(M_{10})) = 0
\end{aligned}
$$

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The expression $m - \mathsf{E}(M_{10})$ is called *bias* - hence *bias-variance decomposition* (which apparently holds in greater generality, not ust for M_{10})

The estimates for which is bias equal to zero - and thence their expected value is equal to the estimated quantity - are called *unbiased*

Is $\mathsf{E}(M_{10}) = m$ - that is, is M_{10} an unbiased estimator of m?

A quick check of bias

```
> mean(replicate(100000,median(rexp(10))))
[1] 0.745127
> median(rexp(100000))
[1] 0.6890036
```

We can see that bias is likely not equal to 0 - even without knowing the exact value

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```
> mm=-log(0.5)
> mm
[1] 0.6931472
```

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We estimated it by 0.6890036, and the difference with 0.745127 seems to be big enough to be just attributed to chance

So M_{10} is apparently not unbiased. However, if we increase n and take M_{100} instead, we can see the situation improving

```
> mean(replicate(100000,median(rexp(100))))
[1] 0.6987744
```

Seems like some consistency holds there...

Back to mean squared error

So, let us do mean squared error now. First, there is a possibility that we actually know an estimated value

```
> mm=-log(0.5)
> mm
[1] 0.6931472
> mean(replicate(10,(median(rexp(10))-mm)^2))
[1] 0.06314839
> mean(replicate(100,(median(rexp(10))-mm)^2))
[1] 0.08828418
> mean(replicate(100,(median(rexp(10))-mm)^2))
[1] 0.1249923
> mean(replicate(100,(median(rexp(10))-mm)^2))
[1] 0.06841089
> mean(replicate(100000,(median(rexp(10))-mm)^2))
[1] 0.09911663
> mean(replicate(100000,(median(rexp(10))-mm)^2))
[1] 0.09856143
> mean(replicate(100000,(median(rexp(10))-mm)^2))
[1] 0.0979045
```

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What if we do not know the estimated value?

Well, then instead of `-log(0.5)` we have to do something else, and if it involves random numbers, we may need to wait a bit longer

```
> mm=median(rexp(10000000))    ## consistency, remember?
> mm
[1] 0.6930446
> mean(replicate(100000,(median(rexp(10))-mm)^2))
[1] 0.09919107
> mean(replicate(100000,(median(rexp(10))-mm)^2))
[1] 0.0988128
> mean(replicate(100000,(median(rexp(10))-mm)^2))
[1] 0.09927002
```

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Confronting with large n approximation

Actually, theory does not help us too much here. The only useful theoretical result concerns M_n for n large. In such a case, M_n is very close to μ, and the mean squared error is thus very close to variance, which in turn can be approximated by

$$\frac{1}{4nf^2(\mu)} \qquad \text{(theorem by Kolmogorov)}$$

where f is the density of the distribution underlying the sample in our case.

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Looks like this not that bad approximation already for $n = 100$

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```
> mm = -log(0.5)
> mean(replicate(100000,(median(rexp(100))-mm)^2))
[1] 0.01004371
> 1/(4*100*dexp(log(2))^2)
[1] 0.01
```

but not that good for $n = 10$ (which is apparently not that large)

```
> 1/(4*10*dexp(log(2))^2)
[1] 0.1      # compare to the Monte Carlo value above
```

A research story

So, we have the estimator, sample median M_{10}, of m

This estimator works in general - for various distributions

say, for the exponential distribution with $\lambda = 1$

or for the exponential distribution with unknown λ

However, when the data follow an exponential distribution

that is, an exponential distribution with unknown λ

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In the latter case, we may actually devise a better estimator for m

How about $Q(0.5)$? Well, actually it is $Q_\lambda(0.5)$

and λ we do not know

but we can estimate it by $1/\bar{X}$

Well, and how do we know it is better?

- well, mean squared error, is it not?

Theory for mean-squared error

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Computer experiment

Let us calculate the mean squared error - in a way that was already shown above - for a couple of selected λ and we will see (as a blind said to a deaf). A tiny script:

```
N <- 100000
n <- 10
las <- c(0.01,0.1,1,10,100)
rslt <- matrix(0,2,length(las))
for (k in (1:length(las))) {
  mm <- qexp(0.5,las[k])
  rslt[1,k] <-
    mean(replicate(N,(median(rexp(n,las[k])) - mm)^2))
  rslt[2,k] <-
    mean(replicate(N,(qexp(0.5,1/mean(rexp(n,las[k]))) - mm)^2))
}
print(rslt)
```

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And the result

```
> source("twomed.R")
         [,1]     [,2]       [,3]         [,4]         [,5]
[1,] 998.0411 9.915687 0.09901681 0.0009827265 9.896574e-06
[2,] 477.9990 4.822185 0.04794337 0.0004825622 4.823859e-06
```

So, we seem to be good...

for five values of λ

and the $N = 100000$ used

and when the data come from an exponential distribution

and if we did not have an error in the code

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An error???

For instance, we could change n to $n = 100$ now

```
> source("twomed.R")
         [,1]      [,2]        [,3]         [,4]         [,5]
[1,] 99.81847 0.9905156 0.009954382 1.010295e-04 9.962715e-07
[2,] 47.99285 0.4794193 0.004777554 4.797323e-05 4.821234e-07
```

and then try the large-sample approximation for the first line

```
> las
[1] 1e-02 1e-01 1e+00 1e+01 1e+02
> 1/(4*100*dexp(qexp(0.5,las),las)^2)
[1] 1e+02 1e+00 1e-02 1e-04 1e-06
```

and for the second one

```
> (-log(0.5)/(las*sqrt(n)))^2
[1] 4.80453e+01 4.80453e-01 4.80453e-03 4.80453e-05 4.80453e-07
```

Seems like we are good...

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Aside: an even a bit better way

```
N <- 100000
n <- 10
las = c(0.01,0.1,1,10,100)
rslt <- matrix(0,2,length(las))
mses <- matrix(0,2,N)
for (k in (1:length(las))) {
  for (rep in 1:N) {
    mm <- qexp(0.5,las[k])
    sss <- rexp(n,las[k])
    mses[1,rep] <- (median(sss) - mm)^2
    mses[2,rep] <- (qexp(0.5,1/mean(sss)) - mm)^2
  }
  rslt[1,k] <- mean(mses[1,])
  rslt[2,k] <- mean(mses[2,])
}
print(rslt)
```

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Not that different results, however

```
> source("twomod.R")
          [,1]     [,2]       [,3]         [,4]         [,5]
[1,] 987.1046 9.903584 0.09875735 0.0009891487 9.820579e-06
[2,] 483.8226 4.801344 0.04818387 0.0004835474 4.800250e-06
```

Recall the earlier

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```
> source("twomed.R")
          [,1]     [,2]       [,3]         [,4]         [,5]
[1,] 998.0411 9.915687 0.09901681 0.0009827265 9.896574e-06
[2,] 477.9990 4.822185 0.04794337 0.0004825622 4.823859e-06
```

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And now for something a bit different

Fine... so the above gave me the mean squared error (which may be close to variance or not) for a sample median out of $n = 10$ *when sampled from the exponential distribution with* $\lambda = 1$

But now I have the following 10 numbers; I compute the median from them - any possibility to assess the precision of that?

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```
> exs
 [1]  2.710660  1.100322 11.934400  1.419022  1.523077
 [6]  5.384740  2.801879  2.163556  4.837161 10.374159
> mm=median(exs)
> mm
[1] 2.75627
> var(exs)
[1] 14.67475
```

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Yes, but does this say anything at all here?

```
> mean((exs-mm)^2)
[1] 15.99159
```

And this one??

Bootstrap!

How about taking the mean squared differences of the sample median of “the sample” (=original batch of numbers) from the sample medians repeatedly calculated... from the data at hand!

```
> mean((replicate(10,median(sample(exs,10)))-mm)^2)
[1] 0
```

Well, if we sample n numbers from n numbers (“resample”), then we always get the same thing; we need to do it *with replacement*

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```
> mean((replicate(10,median(sample(exs,10,replace=TRUE)))-mm)^2)
[1] 2.362092
> mean((replicate(10,median(sample(exs,10,replace=TRUE)))-mm)^2)
[1] 3.502714
> mean((replicate(10,median(sample(exs,10,replace=TRUE)))-mm)^2)
[1] 3.041924
> mean((replicate(100000,median(sample(exs,10,replace=TRUE)))-mm)^2)
[1] 2.125004
> mean((replicate(100000,median(sample(exs,10,replace=TRUE)))-mm)^2)
[1] 2.111911
> mean((replicate(100000,median(sample(exs,10,replace=TRUE)))-mm)^2)
[1] 2.125408
```

The scheme of bootstrap

We are trying to figure out the quantity that may involve

an unknown constant(s) - here let it be just one, m

And also depends on random variables $X_1, \ldots X_n$

independent and with the same distribution

which are believed to be those whose outcomes model the behavior of the observations $x_1, \ldots x_n$ ("sample")

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A *bootstrap estimate* of the desired quantity is then obtained by

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estimating the unknown constant(s) from the original $x_1, x_2, \ldots x_n$

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and then estimating the quantity itself from N batches of n numbers $x^*_{1i}, x^*_{1i} \ldots x^*_{ni}$ sampled from the original $x_1, x_2, \ldots x_n$ *with replacement* ("resampling")

For instance, we are after

$\mathsf{E}\left[(M_{10}(X_1, \ldots, X_{10}) - m)^2\right]$ which we estimate by

$$\frac{1}{N}\sum_{i=1}^{N}\left(M_{10}(x^*_{1i}, \ldots, x^*_{10,i}) - M_{10}(x_1, \ldots, x_{10})\right)^2$$

Excercise: bias, variance

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Bias and variance

We know the sample median is in general biased... Can we obtain the estimate of the bias? (bias = the difference between the estimated value and the expected value of the estimator; equal zero for unbiased estimators)

```
> mm-mean(replicate(10000,median(sample(exs,10,replace=TRUE))))
[1] -0.4691844
```

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What is the variance (may be needed for confidence intervals, say)

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```
> var(replicate(10000,median(sample(exs,10,replace=TRUE))))
[1] 1.895233
```

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Efron & Tibshirani say that 200 would be enough (instead of 10000)... They may be right...

```
> var(replicate(200,median(sample(exs,10,replace=TRUE))))
[1] 1.831597
> var(replicate(200,median(sample(exs,10,replace=TRUE))))
[1] 2.062268
> var(replicate(10000,median(sample(exs,10,replace=TRUE))))
[1] 1.931406
```

And now, hocus-pocus

Bias-variance decomposition again: is it true here?

```
> set.seed(007); mse=mean((replicate(1000000,
+ median(sample(exs,10,replace=TRUE)))-mm)^2)
> mse
[1] 2.116876
> set.seed(007); mvr=var(replicate(1000000,
+ median(sample(exs,10,replace=TRUE))))
> mvr
[1] 1.881946
> set.seed(007); bias=mm-mean(replicate(1000000,
+ median(sample(exs,10,replace=TRUE))))
> bias
[1] -0.4846973
> mvr+bias^2
[1] 2.116877
> mse
[1] 2.116876
```

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If time permits, we may return to cover bootstrap confidence intervals

And again different: permutation tests

We have two batches of 10 numbers:

```
> s1
[1]  3.7551030 11.7892438  4.1296516  0.9881743  1.1722081
[6]  1.1131551  7.5318461  4.9694114  0.6259583  1.3886535
> s2
[1] 1.2574818 1.9363749 1.4094235 0.9201450 2.4456553
[6] 4.9157286 0.7597842 0.5466244 0.7560977 1.5443949
```

Their means turn out to be quite different

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```
> mean(s1)
[1] 3.746341
> mean(s2)
[1] 1.649171
> dss=mean(s1)-mean(s2)
> dss
[1] 2.097169
```

Is this difference significant at level 0.05?

The usual take on it

```
> t.test(s1,s2,alternative="greater")

Welch Two Sample t-test
...
t = 1.7312, df = 11.26, p-value = 0.05534
alternative hypothesis: true difference in means is greater than 0
...
mean of x mean of y
 3.746341  1.649171
```

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```
> t.test(s1,s2,var.equal=TRUE,alternative="greater")
```

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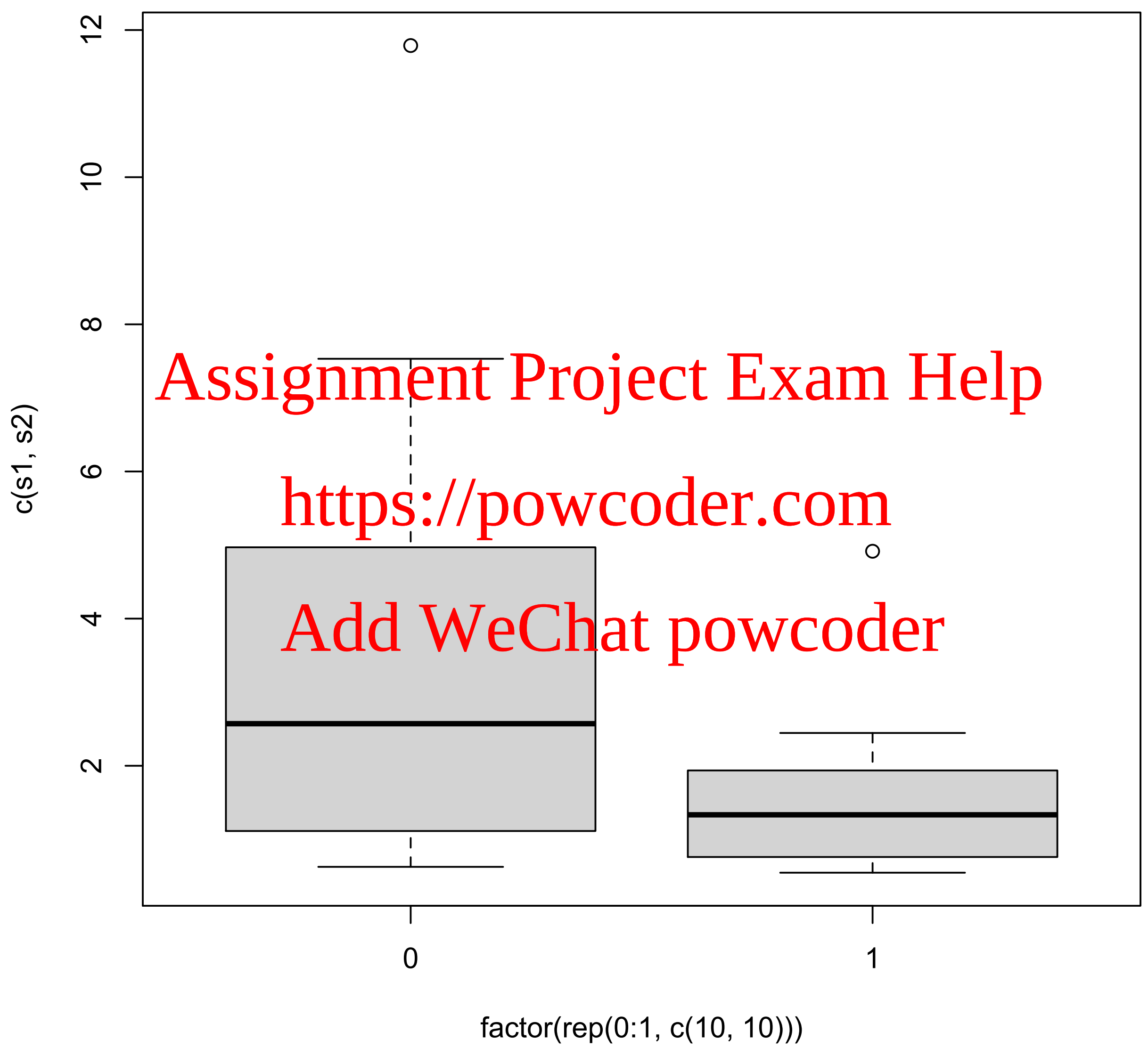
```
Two Sample t-test

t = 1.7312, df = 18, p-value = 0.05026
alternative hypothesis: true difference in means is greater than 0
...
mean of x mean of y
 3.746341  1.649171
```

The underlying assumptions?



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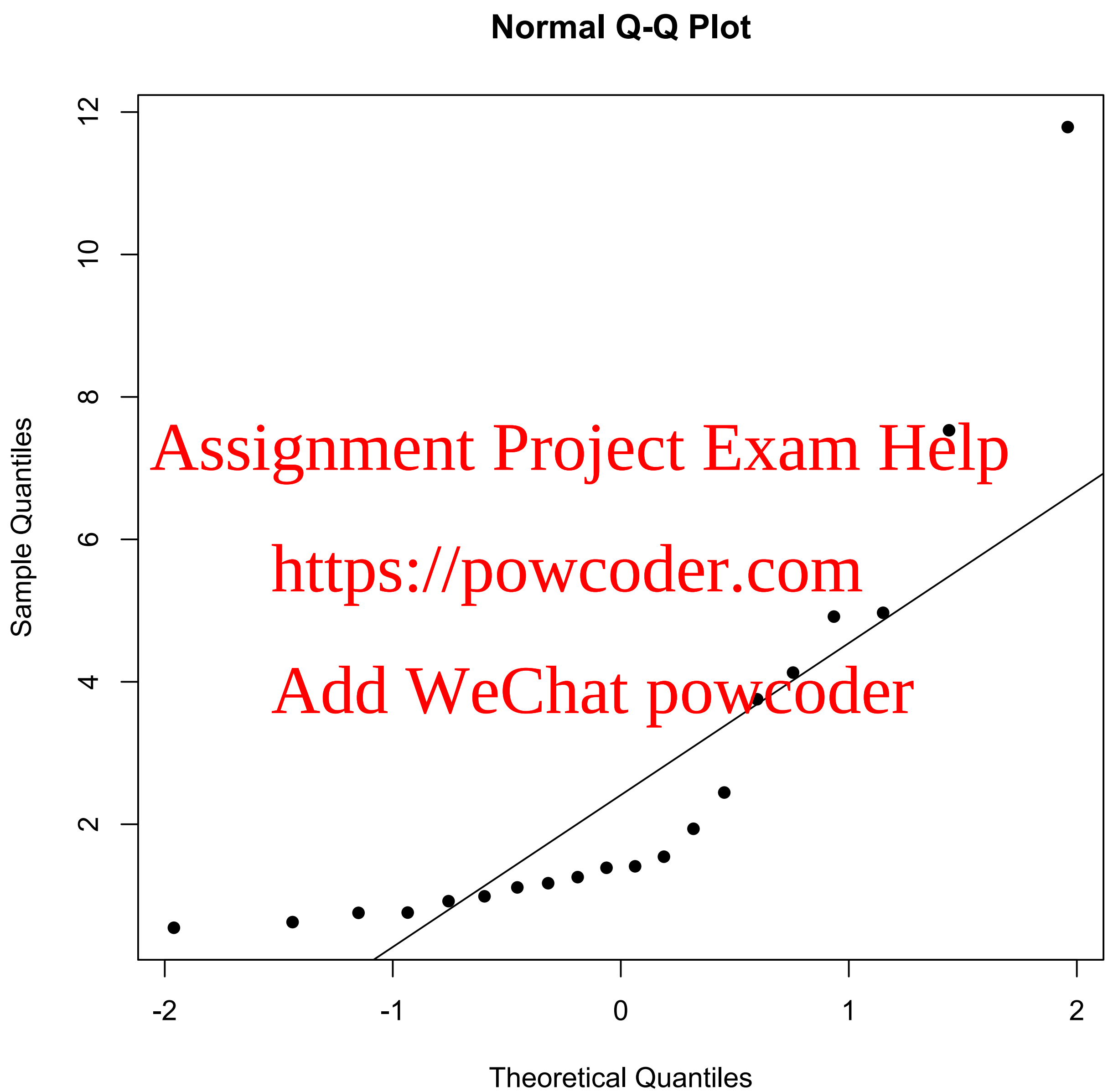
In particular, normality?



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Note: putting both together is a bit tricky here... is it clear why?

Permutation test!

If you think of both as having no difference, you can think about them as that their assignment into `s1` and `s2` is by pure chance: it is then equally likely that they end up as they did, with difference in means `dss = 2.097169` as well as they do other way round, difference in means being then `dss = -2.097169` - and most differences will be around 0 anyway...

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However, the observed difference `dss = 2.097169`: is it not somewhat unlikely? To see that, we could take all possible outcomes under random allocations into `s1` and `s2` - and figure out how many differences of means exceed 2.097169

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That certainly can be done, if we have enough time to wait for the result of $\binom{20}{10}$ allocations... if not, then...

... then we can do just random sampling of those, cannot we?

So, now only how to do it

We first illustrate the code on a very simple numbers - so that we can see what is to be done

```
> s1
[1] 15 16 17 18 19
> s2
[1] 5 6 7 8 9
> s12 = c(s1,s2) ; s12
 [1] 15 16 17 18 19  5  6  7  8  9
> mean(s1)
[1] 17
> mean(s2)
[1] 7
> dss = mean(s1) - mean(s2) ; dss
[1] 10
> sss = sum(s12)/5 ; sss
[1] 24
> sss - 2*mean(s2)      ## this is my trick to have the code short
[1] 10
```

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So, here is what we are going to do

The above was for the observed `s1` and `s2`. Now we combine their values into `s12` and then we are going to sample *new* `s1` and `s2`, again and again. For each of those, we compare the difference of their means with `dss`, the original difference of the means of `s1` and `s2`, and count the proportion of how many times it gets exceeded

```
> sample(s12,5)
[1] 17 16  5  6 19
> sss-2*mean(sample(s12,5))  ## note: sample is different - know why?
[1] 7.6
> replicate(10,sss-2*mean(sample(s12,5)))
 [1]  1.6 -6.0 -5.6  1.6 -1.6 -1.6  3.6  1.2  2.4  5.2
> replicate(10,sss-2*mean(sample(s12,5))) > dss
 [1] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
> mean(replicate(10,sss-2*mean(sample(s12,5))) > dss)
[1] 0   ## also here it could be different, but isn't - guess why
```

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And now with real `s1` and `s2`

```
> s12=c(s1,s2)
> s12
 [1]  3.7551030 11.7892438  4.1296516  0.9881743  1.1722081
 [6]  1.1131551  7.5318461  4.9694114  0.6259583  1.3886535
[11]  1.2574818  1.9363749  1.4094235  0.9201450  2.4456553
[16]  4.9157286  0.7597842  0.5466244  0.7560977  1.5443949
> sss=sum(s12)/10 ; sss
[1] 5.395512
> dss
[1] 2.097169
> mean(replicate(100,sss-2*mean(sample(s12,10))) > dss)
[1] 0.06
> mean(replicate(100,sss-2*mean(sample(s12,10))) > dss)
[1] 0.07
```

Seems like it works now; only $N = 100$ does not yield stable result

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The final run

```
> mean(replicate(100000,sss-2*mean(sample(s12,10))) > dss)
[1] 0.04684
> mean(replicate(100000,sss-2*mean(sample(s12,10))) > dss)
[1] 0.04713
> mean(replicate(100000,sss-2*mean(sample(s12,10))) > dss)
[1] 0.04674
> mean(replicate(100000,sss-2*mean(sample(s12,10))) > dss)
[1] 0.04633
```

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Seems like this is stable enough, and consistently below 0.05 - that is, the test would reject the null hypothesis that there is no difference. We can still give it a final run

```
> set.seed(007)
> mean(replicate(10000000,sss-2*mean(sample(s12,10))) > dss)
```

and when we return after getting a beer from the fridge, we find

```
[1] 0.0467867
```