Lecture 8: Distributions as Models ~~and More Simulations~~

STAT GR5206 *Statistical Computing & Introduction to Data Science*

① Maximum Likelihood Est

② Method of Moments

Gabriel Young
Columbia University

June 20, 2017

Course Notes

- Final Exam: Next Thursday.
- It might be a take home exam.
- Exam details discussed early next week.

Last Time

- **Permutation test**. Testing if two distributions are the same.
- In-class example: Non-parametric version of the two-sample t-test.

This Time

- **Distributions as Models:**
- The Method of Moments
- Maximum Likelihood Estimation

Distributions as Models

Cats

The cats dataset includes the heart and body weights of samples of male and female cats. All the cats are adults and over 2 kg in body weight.

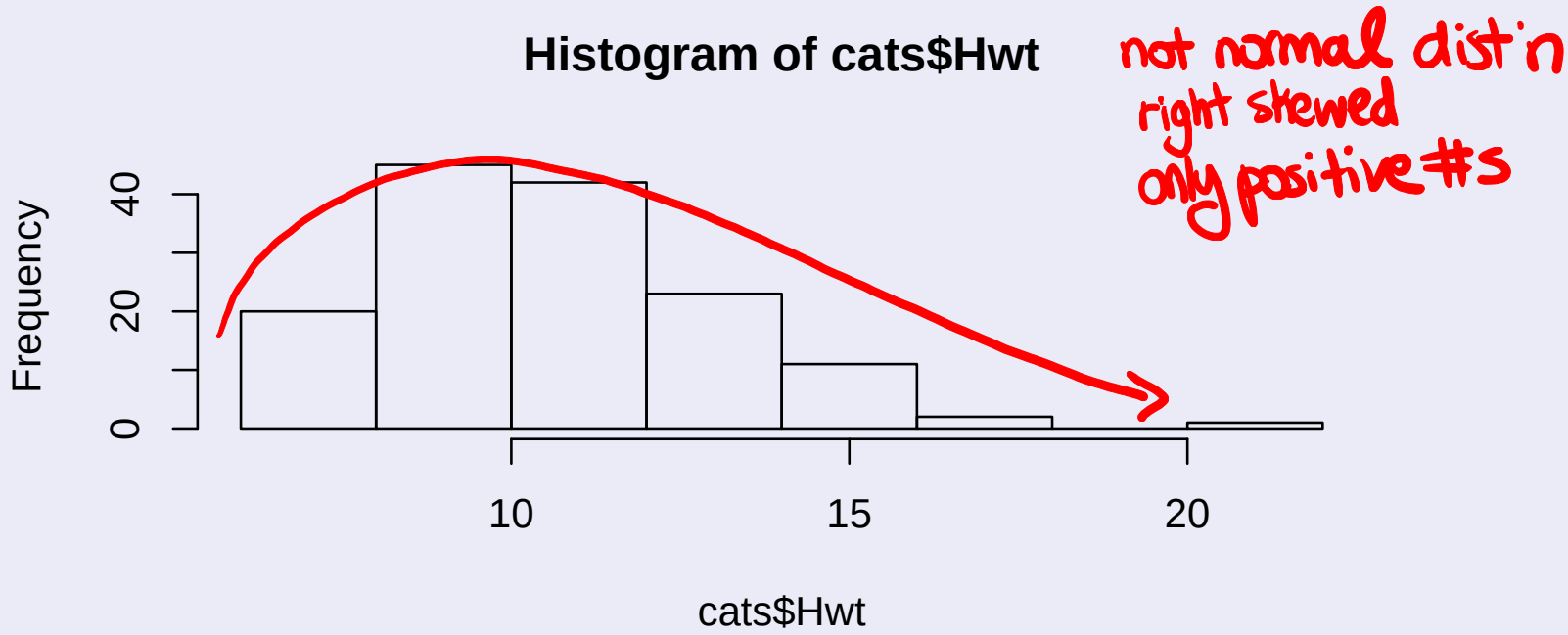
```
> # install.packages("MASS")
> library(MASS)
> head(cats)
```

```
  Sex Bwt Hwt
1   F 2.0 7.0
2   F 2.0 7.4
3   F 2.0 9.5
4   F 2.1 7.2
5   F 2.1 7.3
6   F 2.1 7.6
```

The Distribution of the Data

We've studied how to visually inspect the distribution of a continuous random variable.

```
> hist(cats$Hwt)
```



The Distribution of the Data

R Functions to study the Data's Distribution

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

```
> quantile(cats$Hwt, c(0.25, 0.5, 0.75))
   25%    50%    75%
 8.950 10.100 12.125
```

What % of data lays in which pieces?

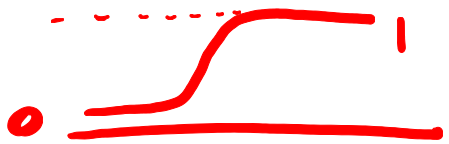
cutoff values

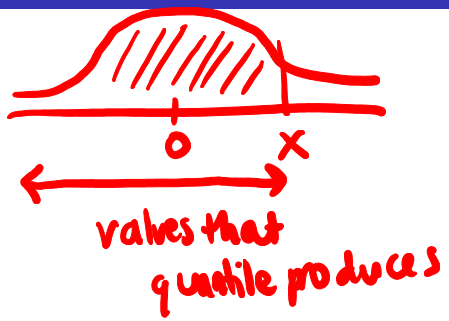
help construct ☐ & whisker plot

The Distribution of the Data

$$f(x) = \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2}x^2\right\}, \quad -\infty < x < \infty$$

$$F(x) = \int_{-\infty}^{x} f(t)\,dt$$





R Functions to study the Data's Distribution

`ecdf()`: **e**mprical **c**umulative **d**istribution **f**unction. No assumptions but also no guess about the distribution beyond the observations.

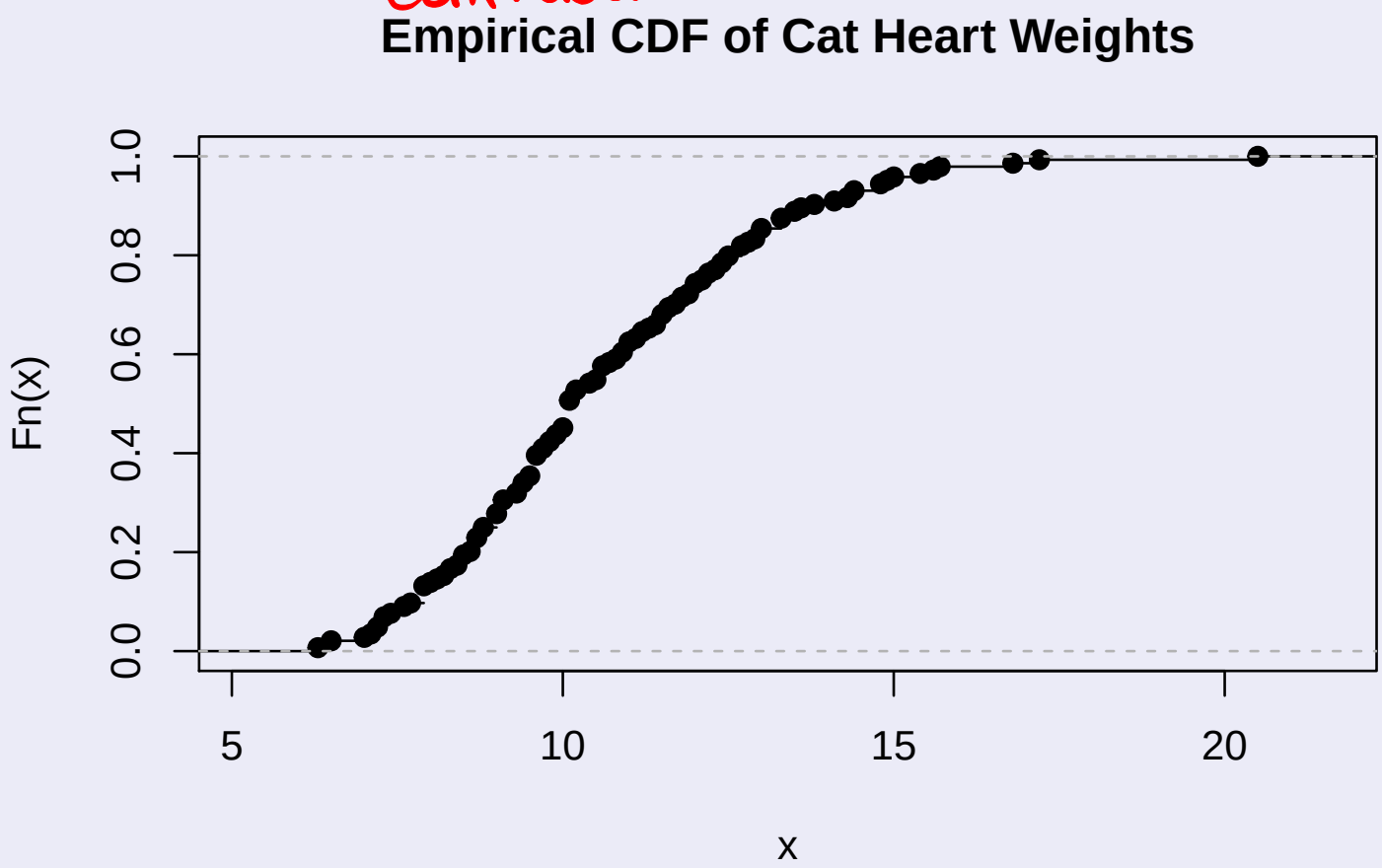
- In math ECDF is written as $\hat{F}$ or $\hat{F}_n$ (n) from data
- Conceptually, `quantile()` and `ecdf()` are inverses to each other.

you can estimate cdf using quantile.

The Distribution of the Data

```
> plot(ecdf(cats$Hwt),
+      main = "Empirical CDF of Cat Heart Weights")
```

continuous distribution



The Distribution of the Data

R Functions to study the Data's Distribution

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

- "Bandwidth" = width of window around each point
- AKA calculates a 'kernal density estimate'
- `density()` returns a collection of x, y values suitable for plotting

ecdf vs density

↳ build plots off of histogram

The Distribution of the Data

R Functions to study the Data's Distribution

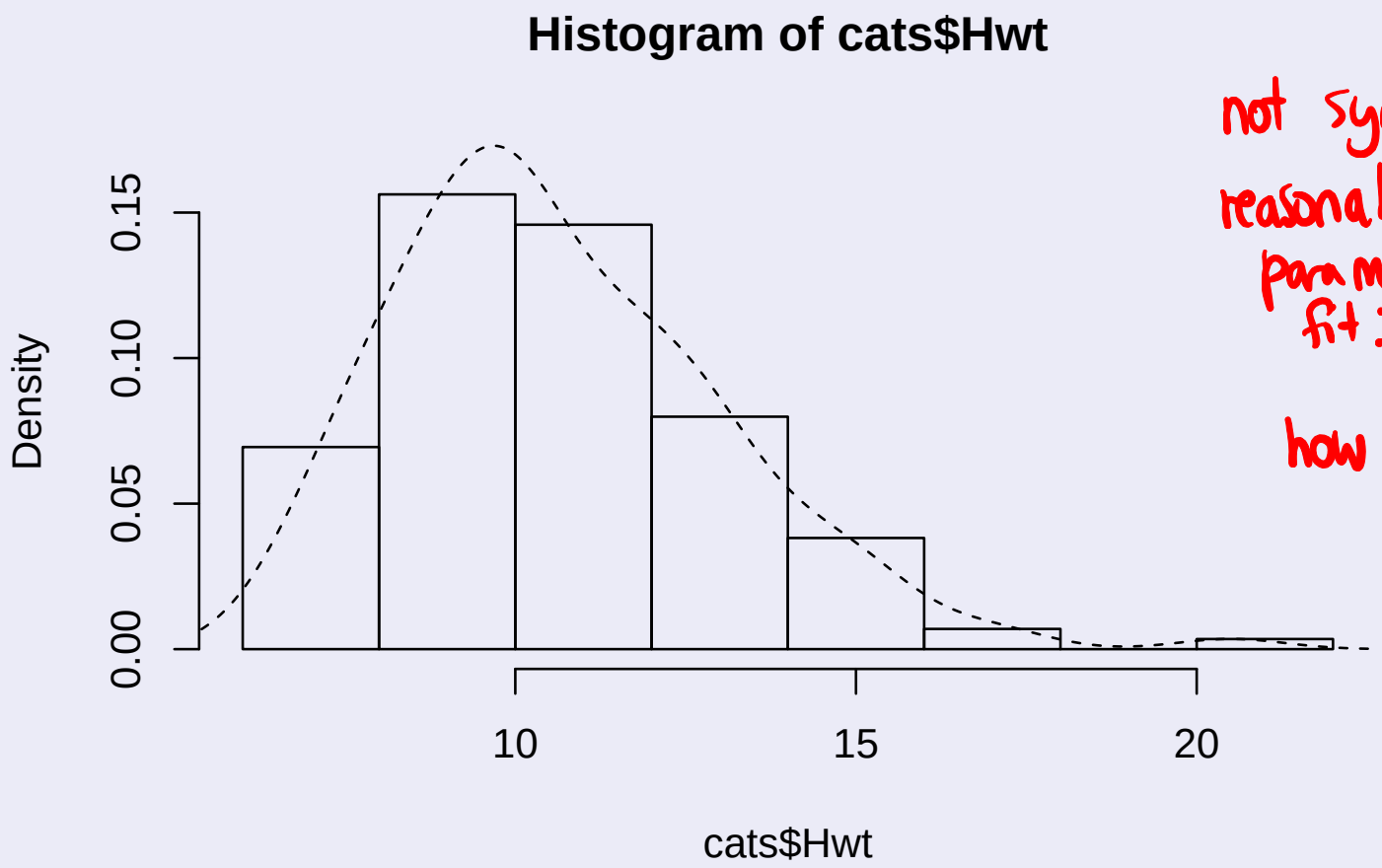
`density(x)`: estimates the density of `x` by counting how many observations fall in a little window around each point, then smoothing.

- "Bandwidth" = width of window around each point
- AKA calculates a 'kernal density estimate'
- `density()` returns a collection of x, y values suitable for plotting

Note, `density()` is an *estimate* of the pdf, not the truth.

The Distribution of the Data

```
> hist(cats$Hwt, probability = TRUE, ylim = c(0, 0.17))
> lines(density(cats$Hwt), lty = "dashed")
```



not symmetric
reasonable parametric fit: gamma

how to fit gamma?

Why Do We Care About the Distribution of the Data?

- The data itself is too much information and *overly detailed*. Don't need to keep around every single data point.
- Plus, the exact data would never repeat itself if we re-sampled anyways.

Why Do We Care About the Distribution of the Data?

- The data itself is too much information and *overly detailed*. Don't need to keep around every single data point.
- Plus, the exact data would never repeat itself if we re-sampled anyways.
- **Goal**: Store information that *summarizes* what will *generalize* to other situations.
    - Can do this by using a model and only keeping the model's parameters.

How Do We Fit Distributional Models to Data?

Recall that most models are defined by *parameters* (like (μ, σ^2) for the normal). So *fitting* a model to data means finding those parameters such that the model best fits the data.

How Do We Fit Distributional Models to Data?

Recall that most models are defined by *parameters* (like (μ, σ^2) for the normal). So *fitting* a model to data means finding those parameters such that the model best fits the data.

- Match moments (mean, variances, etc.). Method of Moments *
- Match other summary statistics.
- Maximize the likelihood.

$\int x^n f(x)\,dx = E[X^n] = n^{th}$ moment of rv X

$E[(X - EX)^n] = n^{th}$ central moment of X

2nd central moment = variance

Recall the Gamma Distribution

- The **gamma** distributions are a family of probability distributions defined by the density functions,

continuous factorial * $\Gamma(a) = \int_0^\infty x^{a-1} e^{-x} dx$

$$f(x) = \frac{x^{a-1} e^{-x/s}}{s^a \Gamma(a)}, \quad x > 0$$

where the gamma function $\Gamma(a) = \int_0^\infty u^{a-1} e^{-u} du$ is chosen so that the total probability of all non-negative x is 1.

- Parameter a ($a = \alpha$) is the **shape**, and s ($s = \beta$) is the **scale**.
- The expected value is as, and the variance as^2.

Method of Moments

2 moments:
sample mean = True mean sample variance = True variance

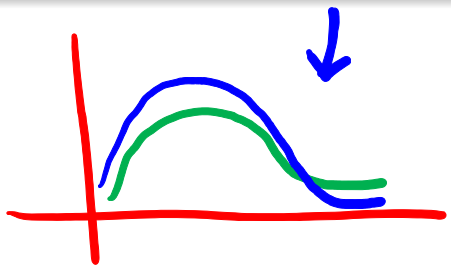
- Pick enough moments that they *identify* the parameters. At least one moment per parameter. (mean, var)
- Write equations for the moments in terms of the parameters.
  - E.g. for gamma,

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

- Solve the moment equations for the parameters (usually done by hand).
  - E.g. for gamma,

$$a = \frac{\mu^2}{\sigma^2}, \quad s = \frac{\sigma^2}{\mu}.$$

sample values that will fit function into gamma



Check Yourself

Tasks

- Write a function `gamma.MMest` that takes as input a data vector and returns estimates of the scale parameters a and s using the moment equations from the previous slide.
- Plug cat heart weights into your function to get estimates of a and s.

```
gamma.MMest <- function(vec){
    a <- mean(vec)^2/var(vec)
    s <- var(vec)/mean(vec)
    return(c(a,s))
}
```

Check Yourself

Tasks

- Write a function `gamma.MMest` that takes as input a data vector and returns estimates of the scale parameters a and s using the moment equations from the previous slide.
- Plug cat heart weights into your function to get estimates of a and s.

Tasks

```
> gamma.MMest <- function(data) {
+   m <- mean(data)
+   v <- var(data)
+   return(c(a = m^2/v, s = v/m))
+ }
```

Check Yourself

Tasks

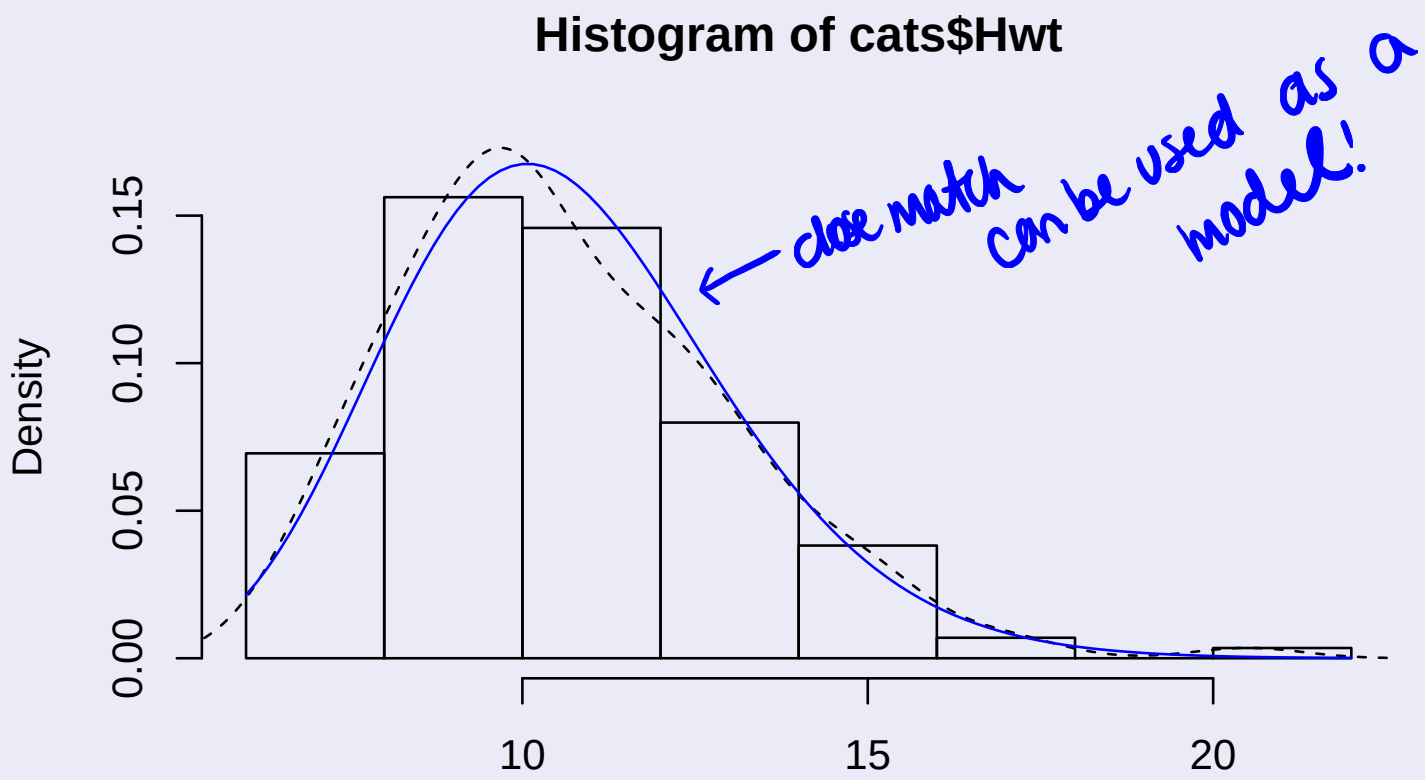
- Write a function `gamma.MMest` that takes as input a data vector and returns estimates of the scale parameters a and s.
- Plug cat heart weights into your function to get estimates of a and s.

Tasks

```
> gamma.MMest(cats$Hwt)

         a          s
19.0653121  0.5575862
```

Method of Moments

```
> hist(cats$Hwt, probability = TRUE, ylim = c(0, 0.17))
> lines(density(cats$Hwt), lty = "dashed")
> cat.MM <- gamma.MMest(cats$Hwt)
> curve(dgamma(x, shape = cat.MM["a"], scale = cat.MM["s"]),
+       add = TRUE, col = "blue")
```



Method of Moments

- Sometimes we can't solve the moment equations for the parameters by hand. In that case, do it numerically.
- Set up a difference function between the data and the model and then minimize this function.

Method of Moments

$Q(a,s) = (\text{mean}(data) - as)^2 + (\text{var}(data) - as^2)^2$

↑ Least Squares Problem!

- Sometimes we can't solve the moment equations for the parameters by hand. In that case, do it numerically.
- Set up a difference function between the data and the model and then minimize this function.

Cats Example

```
> gamma.mean <- function(a, s) {return(a*s)}
> gamma.var  <- function(a, s) {return(a*s^2)}
> gamma.diff <- function(params, data) {
+   a <- params[1]
+   s <- params[2]
+   return((mean(data) - gamma.mean(a,s))^2
+          + (var(data) - gamma.var(a,s))^2)
+ }
```

apply(matrix, 2, mean, trm.NA = True)

Method of Moments

- Sometimes we can't solve the moment equations for the parameters by hand. In that case, do it numerically.
- Set up a difference function between the data and the model and then minimize this function.

Cats Example

```
> nlm(gamma.diff, c(19, 1), data = cats$Hwt)[1:3]

$minimum
[1] 1.899648e-13

$estimate
[1] 19.0653140  0.5575862

$gradient
[1] -5.33881e-09 -2.11992e-07
```

More generally...

Cats Example

- Nothing special about moments. Could match other data summaries too.
  - Examples: the median, quantiles...
- Try to solve for parameters exactly by hand. If you can't set up a discrepancy function and minimize it.

More generally...

Cats Example

- Nothing special about moments. Could match other data summaries too.
  - Examples: the median, quantiles...
- Try to solve for parameters exactly by hand. If you can't set up a discrepancy function and minimize it.
- Just make sure your summaries converge to the population values.
  - How? Simulate then estimate and estimates should converge as the sample grows.

Check Yourself: Checking Your Estimator

Task

- Simulate 100 random variables from a gamma distribution with shape parameter equal to 19 and scale parameter equal to 45. Run the `gamma.MMest` with these values as the input.
- Do the same thing but simulate $10,000$ random variables. Next, $1,000,000$ random variables.
- Does it seem like our estimates are converging to the truth?

Check Yourself: Checking Your Estimator

Solutions

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

       a        s
18.13141 47.33718

> gamma.MMest(rgamma(10000, shape = 19, scale = 45))

       a        s
18.91902 45.07275

> gamma.MMest(rgamma(1000000, shape = 19, scale = 45))

       a        s
19.00058 45.01128
```

numerically consistent estimators

Maximum Likelihood

- Usually we think of parameters, θ, as fixed and consider the probability of different outcomes $f(x, \theta)$ with θ constant and x changing.

Prob density $= f(x) = f(x; \theta)$

$= f_\theta(x)$

$= f(x \mid \theta)$

function of x

Maximum Likelihood

- Usually we think of parameters, θ, as fixed and consider the probability of different outcomes $f(x, \theta)$ with θ constant and x changing.
- **Likelihood** of a parameter value is given by $L(\theta)$: what probability does θ give the data?
  - For continuous variables, use the probability density.
  - Calculate $f(x, \theta)$ letting θ change with data constant.
  - *Not* the probability of θ.

Maximum Likelihood

↑ function of parameter

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

Likelihood $L(\theta) = f(x_1, \dots x_n | \theta)$ ← function of θ

Joint pdf $f(x_1 \cdots x_n | \theta) = f(x_1|\theta) \cdot f(x_2|\theta) \cdots f(x_n|\theta)$

If events A, B are independent.

$\Rightarrow P(A \text{ and } B) = P(A)P(B)$

Random Sample: $X_1, \dots, X_n$ are independent and identically distributed

$f(x_1, \dots, x_n) = f(x_1)f(x_2)\dots f(x_n)$

Coding the Likelihood Function

- With independent data points $x_1, x_2, \ldots, x_n$ the likelihood is

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

- Multiplying lots of small numbering is bad, so we usually take the log:

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

we only care about optimizing θ

- Note the maximizer is the same for both (though the maximum value will be different).

Check Yourself

Tasks

- Write a function `gamma.ll` which takes as input a parameter vector (with shape and scale) and a data vector and from that returns the log likelihood assuming the data are independent draws from a gamma distribution with scale and shape indicated by the input parameter vec. HINT: Use `dgamma()`.
- Test your function on the cats heart weight data and parameter values scale equals 19 and shape equals 0.5.

Check Yourself

Solution

```
> gamma.ll <- function(params, data) {
+   a <- params[1]
+   s <- params[2]
+   return(sum(dgamma(data, shape = a,
+                     scale = s, log = TRUE)))
+ }
> gamma.ll(c(19, 0.05), cats$Hwt)
[1] -21598.19
```

takes log of every single point

only 1 dgamma b/c doing this for n cases

pdf evaluated at data points

How do we maximize the likelihood?

How do we maximize it?

- Sometimes, like for the normal distribution, we can do this by hand with calculus.
- Other times we need to use numerical methods... *minimize* the negative log likelihood.

How do we maximize the likelihood?

How do we maximize it?

- Sometimes, like for the normal distribution, we can do this by hand with calculus.
- Other times we need to use numerical methods... *minimize* the negative log likelihood.

```
> nlm(gamma.ll, c(19, 1), data = cats$Hwt)[1:3]

$minimum
[1] -1334280770

$estimate
[1] 409228.0 469356.4

$gradient
[1] -3404.4834  -125.5524
```

→ not what we want (we want max)

Fix: put negative infront of gamma.ll

How do we maximize the likelihood?

```
> neg.gamma.ll <- function(params, data) {
+   a <- params[1]
+   s <- params[2]
+   return(-sum(dgamma(data, shape = a,
+                      scale = s, log = TRUE)))
+ }
> nlm(neg.gamma.ll, c(19, 1), data = cats$Hwt)$minimum

[1] 325.5476

> nlm(neg.gamma.ll, c(19, 1), data = cats$Hwt)$estimate

[1] 20.299930  0.523674
```

How do we maximize the likelihood?

```
> neg.gamma.ll <- function(params, data) {
+   a <- params[1]
+   s <- params[2]
+   return(-sum(dgamma(data, shape = a,
+                      scale = s, log = TRUE)))
+ }
> nlm(neg.gamma.ll, c(19, 1), data = cats$Hwt)$minimum

[1] 325.5476
```

⇒ max likelihood

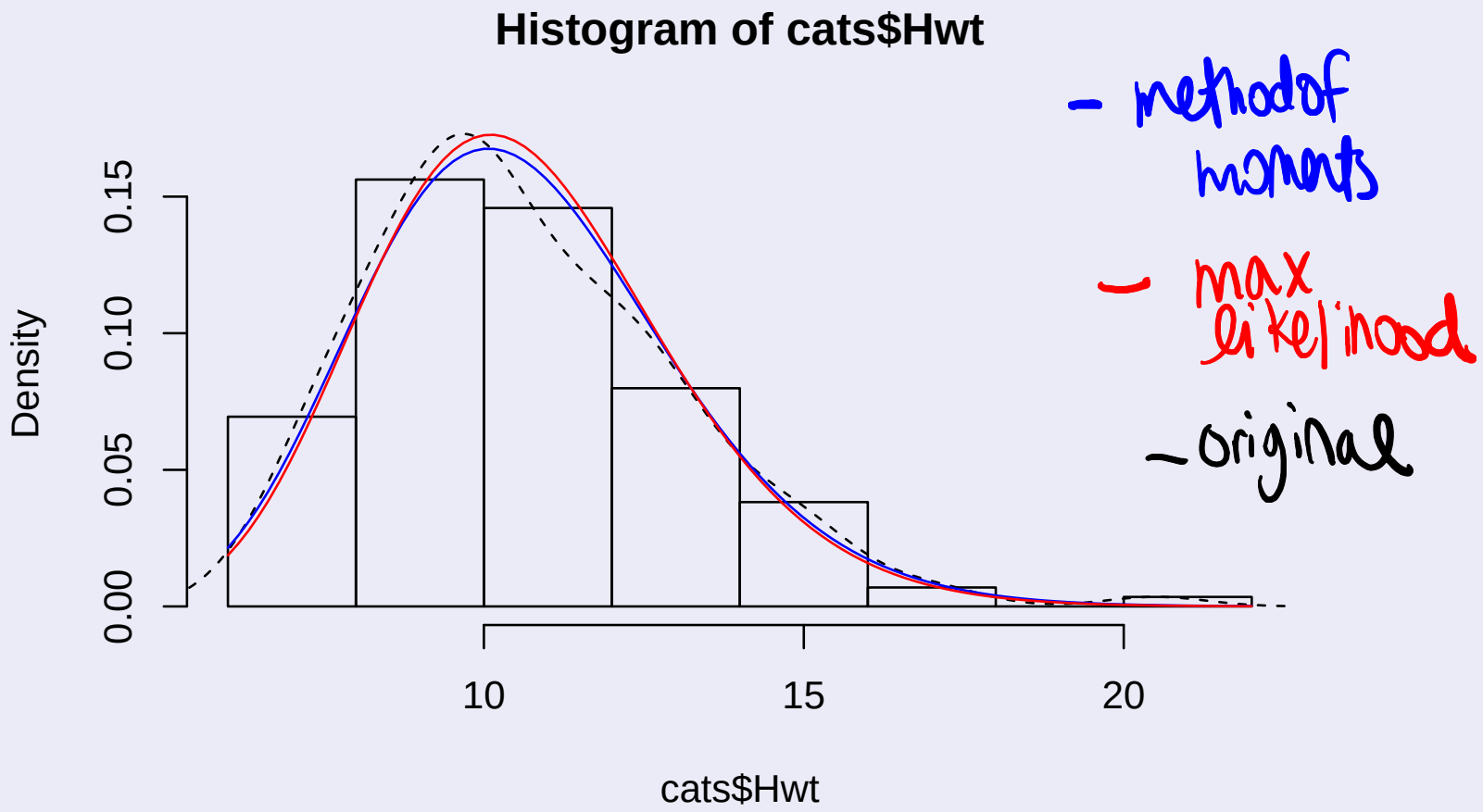
```
> nlm(neg.gamma.ll, c(19, 1), data = cats$Hwt)$estimate

[1] 20.299930  0.523674

> cat.MM <- gamma.MMest(cats$Hwt)
> neg.gamma.ll(cat.MM, cats$Hwt)

[1] 325.6886
```

→ while it does not quite get it. It is very close.

Maximum Likelihood

```
> hist(cats$Hwt, probability = TRUE, ylim = c(0, 0.17))
> lines(density(cats$Hwt), lty = "dashed")
> cat.MLE <- nlm(neg.gamma.ll, c(19, 1), data = cats$Hwt)$estimate
> curve(dgamma(x, shape = cat.MM["a"], scale = cat.MM["s"]),
+       add = TRUE, col = "blue")
> curve(dgamma(x, shape = cat.MLE[1], scale = cat.MLE[2]),
+       add = TRUE, col = "red")
```

Maximum Likelihood



Why the MLE?

- Usually *consistent*: converges to the truth as we get more data.
- Usually *efficient*: converges to the truth as least as fast as anything else.

↳ don't need as much data to converge to truth

Checking Fit

- Plot the data with your estimates (like in the last slide).
- Calculate summary statistics not used in fitting and compare with those of the fitted model.
    - Some plotting tools to help with this.
- Use statistical tests.

Checking Fit: Summary Statistics

```
> # Model quantiles
> qgamma(c(0.01, 0.05, 0.95, 0.99), shape = cat.MM["a"],
+        scale = cat.MM["s"])

[1]  5.795333  6.966974 14.926292 17.097730
> # Data quantiles:
> quantile(cats$Hwt, c(0.01, 0.05, 0.95, 0.99))

    1%     5%    95%    99%
 6.500  7.300 14.885 17.028
```

↳ cut off from gamma curve (theoretical)

↳ cut off from histogram (true)

Checking Fit: Summary Statistics

Quantile-Quantile (Q-Q) Plots

- Plots theoretical vs. actual quantiles.
- Ideally, a straight line when the distributions are the same.
- `qqnorm()` and `qqline()` are specialized for checking normality.
- Could also plot quantiles of two samples against each other.
- `qqplot(x,y)` gives a Q-Q plot of one vector against another.

Checking Fit: Summary Statistics

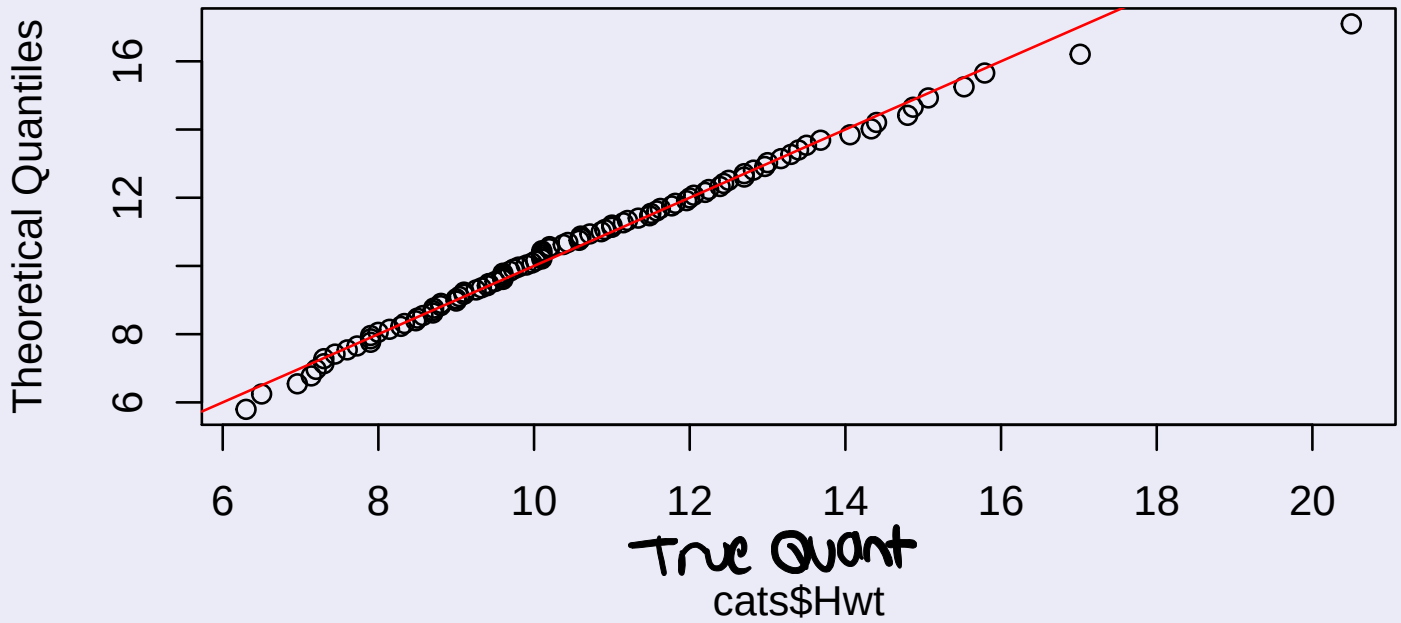
Quantile-quantile Plot

```
> a <- cat.MM["a"]; s <- cat.MM["s"]
> qqplot(cats$Hwt, qgamma((1:99)/100, shape = a, scale = s),
+        ylab = "Theoretical Quantiles")
> abline(0, 1, col = "red")
```

→ method of moments est

→ qq plot

↳ if true quantile = theoretical quantile line should be $y = x$



Checking Fit: Summary Statistics

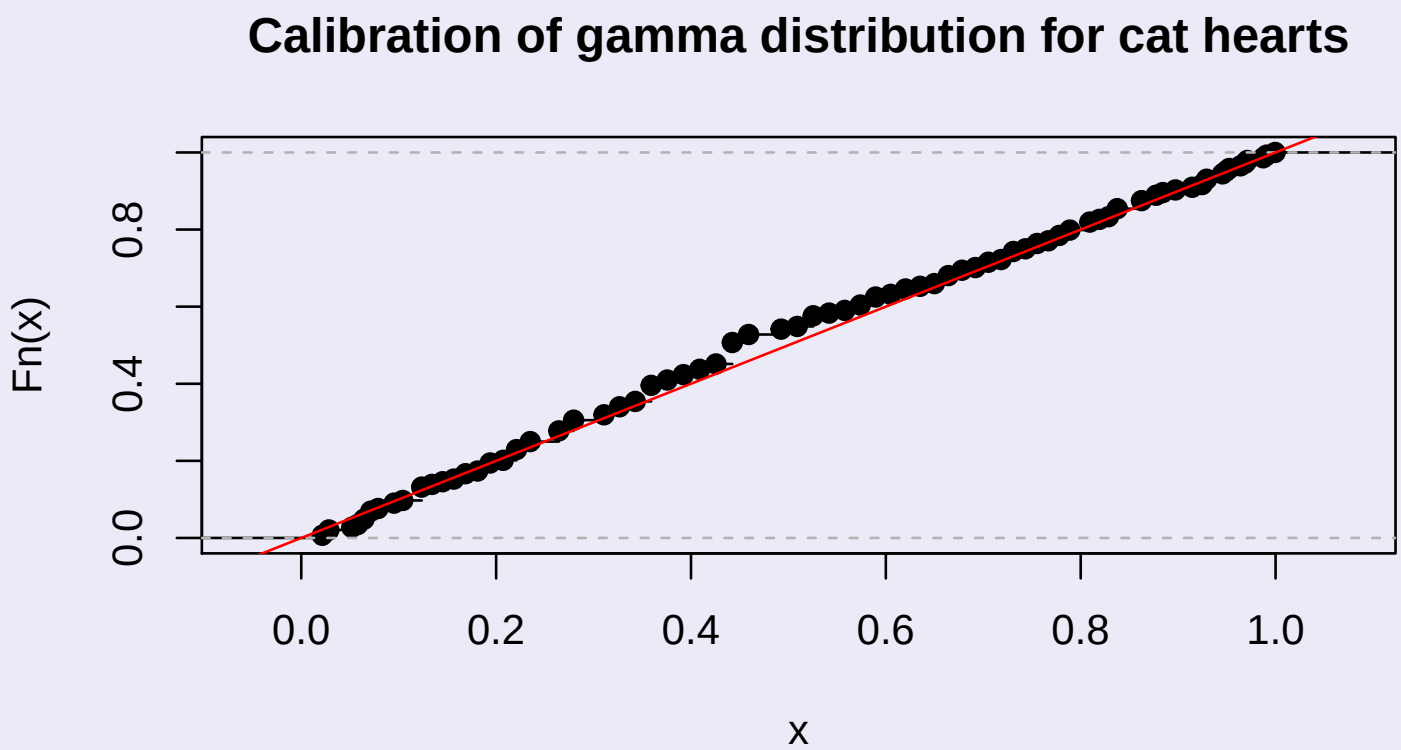
Calibration Plots

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

Checking Fit: Summary Statistics

Cailbration Plots

```
> plot(ecdf(pgamma(cats$Hwt, shape = a, scale = s)),
+         main = "Calibration of gamma distribution for cat hearts")
> abline(0, 1, col = "red")
```



Checking Fit: Kolmogorov-Smirnoff Test

- How much should Q-Q or calibration plot wiggle around the diagonal?

Checking Fit: Kolmogorov-Smirnoff Test

Null Hypothesis

H_0 : $X \sim$ distn

H_1 : X not distn

- How much should Q-Q or calibration plot wiggle around the diagonal?
- Answer a different question: define the biggest gap between theoretical and empirical CDF

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

True Empirical

- D_{KS} always has the same distribution *if* the theoretical CDF is fixed and correct.
- Also works for comparing empirical CDF of two samples to see if they come from the same distribution.

Checking Fit: Kolmogorov-Smirnoff Test

Built in Function!

```
> ks.test(cats$Hwt, pgamma, shape = a, scale = s)

One-sample Kolmogorov-Smirnov test


data:  cats$Hwt
D = 0.0686, p-value = 0.5062
alternative hypothesis: two-sided
```

H_0 : X ~ gamma ✓

H_1 : X not gamma

p-value = .5 $> \alpha$ => Fail To Reject H_0

most likely gamma distn

Checking Fit: Kolmogorov-Smirnoff Test

Warning

- More complicated and not properly handled by built-in `R` if parameters are estimated by the data.
  - Fit looks better than it really is.
- Hack: estimate the model using 90% of the data and check the fit using the K-S test using the other 10% (feels a little bit like *cross*-validation).

Checking Fit: Kolmogorov-Smirnoff Test

```
> n      <- length(cats$Hwt)
> train  <- sample(1:n, size = round(.9*n))
> cat.MM <- gamma.MMest(cats$Hwt[train])
> a <- cat.MM["a"]
> s <- cat.MM["s"]
> a
       a
18.65791
> s
        s
0.5707621
```

Checking Fit: Kolmogorov-Smirnoff Test

```
> ks.test(cats$Hwt[-train], pgamma, shape = a, scale = s)

One-sample Kolmogorov-Smirnov test

data:  cats$Hwt[-train]
D = 0.1856, p-value = 0.6547
alternative hypothesis: two-sided
```

Using Trained model with Test data.

Checking Fit: Kolmogorov-Smirnoff Test

Can also test whether two samples come from the same distribution.

```
> ks.test(cats$Hwt[cats$Sex == "F"],
+         cats$Hwt[cats$Sex == "M"])

Two-sample Kolmogorov-Smirnov test

data:  cats$Hwt[cats$Sex == "F"] and cats$Hwt[cats$Sex == "M"]
D = 0.4942, p-value = 3.847e-07
alternative hypothesis: two-sided
```

→ small pvalue

reject null

not same as female.