James M. Flegal

# Agenda

- Random number generation
- ▶ Distributions in R
- Distributional Models
- ► Moments, generalized moments, likelihood
- Visual comparisons and basic testing

### Random number generation

- ► How does R get "random" numbers?
  - ▶ It doesn't, instead it uses pseudorandom numbers that we hope are indistinguishable from random numbers
  - Pseudorandom generators produce a deterministic sequence that is indistinguishable from a true random sequence if you don't know how it started
  - Why? Truly random numbers are expensive

## Random number generation

- Pseudorandom generators produce a sequence of Uniform(0,1) random variates
- ► Linear congruential generator is one of the oldest and best-known pseudorandom number generator algorithms
- Other distributions usually based such a sequence
- ▶ Example: If  $U \sim \text{Unif}(0,1)$  then  $-\beta \ln(1-U) \sim \text{Exp}(\beta)$
- ▶ More on this later . . .

# Example: runif()

## [7] 0.27453052 0.27230507 0.61582931 0.42967153

```
runif(1:10)

## [1] 0.44083639 0.64647956 0.67560056 0.49333730 0.61593355 0.92339429
## [7] 0.45539437 0.17013010 0.09595561 0.84816697

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

## [1] 0.50747820 0.30676851 0.42690767 0.69310208 0.08513597 0.22543662
```

- ► Easily implemented and fast
- Modulo arithmetic via storage-bit truncation
- Defined as

$$X_{n+1} = (aX_n + c) \mod m$$

where X is the sequence of pseudorandom values

```
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</pre>
```

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

▶ Unfortunately, this sequence has period 8

variates

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

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

```
variates <- rep (NA, out.length)
for (kk in 1:out.length) variates[kk] <- new.random(a=1664545, c=1013904223, m=2^32)
variates

## [1] 1037207853 2090831916 4106096907 768378826 3835752553 1329121000
## [7] 2125006663 2668506502 3881687205 2079234980 2067291011 2197025090
## [13] 3748878561 2913996384 758844863 4029469438 2836748829 1458315036
## [19] 2399149563 2766656186</pre>
```

# How to distinguish non-randomness?

- Look at period
- Missing some values
- Proper distribution in the limit
- Autocorrelation
- Gets harder for higher dimensions

- Beta, Binomial, Cauchy, Chi-Square, Exponential, F, Gamma, Geometric, Hypergeometric, Logistic, Log Normal, Negative Binomial, Normal, Poisson, Student t, Studentized Range, Uniform, Weibull, Wilcoxon Rank Sum Statistic, Wilcoxon Signed Rank Statistic
- ▶ Parameters of these distributions may not agree with textbooks
- Lots of distributions, but they all work the same way

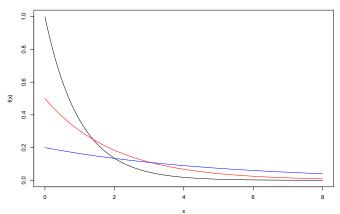
Every distribution that R handles has four functions. There is a root name, for example, the root name for the normal distribution is norm. This root is prefixed by one of the letters

- p for "probability", the cumulative distribution function (c. d. f.)
- q for "quantile", the inverse c. d. f.
- ▶ d for "density", the density function (p. f. or p. d. f.)
- r for "random", a random variable having the specified distribution

- Beta, Binomial, Cauchy, Chi-Square, Exponential, F, Gamma, Geometric, Hypergeometric, Logistic, Log Normal, Negative Binomial, Normal, Poisson, Student t, Studentized Range, Uniform, Weibull, Wilcoxon Rank Sum Statistic, Wilcoxon Signed Rank Statistic
- beta, binom, cauchy, chisq, exp, f, gamma, geom, hyper, logis, lnorm, nbinom, norm, pois, t, tukey, unif, weibull, wilcox, signrank
- Exponential distribution has pexp, qexp, dexp, and rexp

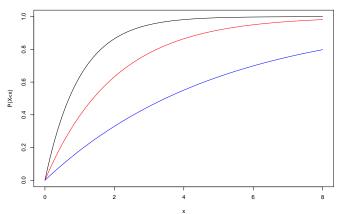
# Exponential distribution

#### **Exponential Distributions**



# Exponential distribution

#### **Exponential Distributions**



# Fitting distributional models

- Method of moments
- Match other summary statistics
- Maximize likelihood estimation

### Method of moments: Closed form

- Pick enough moments to identify the parameters, i.e. at least 1 moment per parameter
- ▶ Write moment equations in terms of the parameters, e.g. the gamma distribution

$$\mu = as \text{ and } \sigma^2 = as^2$$

Solve the system of equations (by hand)

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

Write a function

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

# Method of moments: 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))^2)
}</pre>
```

Minimize your function

# Applies more generally

- Can match other data summaries, e.g. the median or ratios of quantiles
- If you can't solve exactly, set up a discrepancy function and minimize it

### Maximum Likeihood

- ▶ Usually think of parameters as fixed and consider the probability of different outcomes,  $f(x|\theta)$  with  $\theta$  constant and x changing
- ▶ Likelihood of a parameter value, i.e.  $L(\theta)$  treats this a function of  $\theta$
- $\blacktriangleright$  Search over values of  $\theta$  for the one that makes the data most likely
- Results in maximum likelihood estimate (MLE)

### Maximum Likeihood

▶ Suppose  $x_1, ..., x_n$  are i.i.d., then

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

- Tends to be computationally unstable since it may contain lots of small numbers
- Instead consider the log likelihood

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

▶ In pseudo-code

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

### What to do with the likelihood?

- Maximize it!
- Sometimes we can do the maximization by hand via calculus
  - Gaussian, Poisson, Pareto, . . .
- More generally we'll consider numerical optimization
  - ▶ Include a minus sign when using a minimization function

# Why use an MLE?

- Usually consistent: converges on the truth as we get more data
- Usually efficient: converges on the truth at least as fast as anything else
- Some settings where the maximum isn't well-defined (e.g.  $x_{min}$  for a Pareto)
- Sometimes data is too aggregated or mangled to use an MLE

### MLEs for univariate distributions

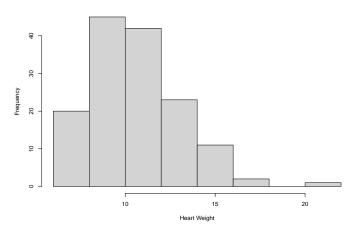
- fitdistr in MASS package
- Knows most standard distributions, but can also handle arbitrary probability density functions
- Starting value for the optimization is optional for some distributions, required for others (including user-defined densities)
- Returns parameter estimates and standard errors from large-n approximations (so use cautiously)

# Example: Cat heart weights

#### library(MASS)

```
## Warning: package 'MASS' was built under R version 4.0.2
data("cats",package="MASS")
hist(cats$Hwt, xlab="Heart Weight", main="Histogram of Cat Heart Weights")
```

#### **Histogram of Cat Heart Weights**

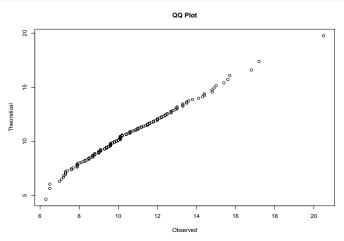


# Example: Cat heart weights

#### fitdistr(cats\$Hwt, densfun="gamma")

```
## shape rate
## 20.2998092 1.9095724
## ( 2.3729250) ( 0.2259942)
```

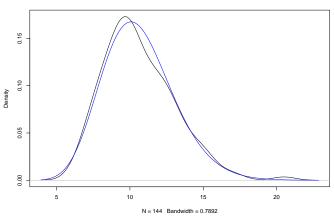
# Checking the fit



# Checking the fit

```
plot(density(cats$Hwt)) # more on this later
curve(dgamma(x,shape=cats.gamma["shape"],scale=cats.gamma["scale"]),add=TRUE,col="blue")
```





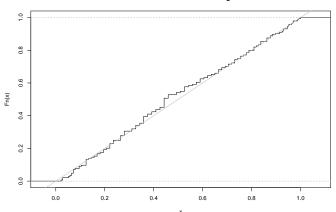
# Calibration plots

- ▶ 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
- Can look at calibration 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

# Calibration plots

```
plot(ecdf(pgamma(cats$Hwt, shape=cats.gamma["shape"], scale=cats.gamma["scale"])),
    main="Calibration Plot for Cat Heart Weights", verticals = T, pch = "")
abline(0,1,col="grey")
```

#### Calibration Plot for Cat Heart Weights



# Calibration plots

Exercise: Write a general function making a calibration plot that inputs a data vector, cumulative probability function, and parameter vector

# Kolmogorov-Smirnov test

- ► How much "error" is acceptable in a QQ plot or calibration plot?
- Alternatively, consider the biggest gap between theoretical and empirical CDF:

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

- Useful because D<sub>KS</sub> has the same distribution if the theoretical CDF is fixed and correct
- Also works for comparing the empirical CDFs of two samples, to see if they came from the same distribution

# Kolmogorov-Smirnov test

```
ks.test(cats$Hwt, pgamma, shape=cats.gamma["shape"], scale=cats.gamma["scale"])

## Warning in ks.test(cats$Hwt, pgamma, shape = cats.gamma["shape"], scale =
## cats.gamma["scale"]): ties should not be present for the Kolmogorov-Smirnov test

##

## One-sample Kolmogorov-Smirnov test

##

## data: cats$Hwt

## D = 0.068637, p-value = 0.5062

## alternative hypothesis: two-sided
```

- Caution: Solution is 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
- ► Could estimate using (say) 80% of the data, and then check the fit on the remaining 20%

# Kolmogorov-Smirnov test

Can also test whether two samples come from same distribution

```
x <- rnorm(100, mean=0, sd=1)
y <- rnorm(100, mean=.5, sd=1)
ks.test(x, y)</pre>##
```

```
##
## Two-sample Kolmogorov-Smirnov test
##
## data: x and y
## D = 0.28, p-value = 0.0007873
## alternative hypothesis: two-sided
```

# Chi-squared test

 Compare an actual table of counts to a hypothesized probability distribution

```
M \leftarrow as.table(rbind(c(762, 327, 468), c(484, 239, 477)))
dimnames(M) <- list(gender = c("F", "M"), party = c("Democrat", "Independent", "Republican"))</pre>
М
         party
## gender Democrat Independent Republican
##
                762
                             327
                                         468
                484
                             239
##
                                         477
Xsq <- chisq.test(M)</pre>
Xsq
##
   Pearson's Chi-squared test
##
## data: M
## X-squared = 30.07, df = 2, p-value = 2.954e-07
```

### Chi-squared test

- ➤ 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

- ▶ 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</pre>
```

```
## [1] 6 8 10 12 14 16 18 20 22 cats.hist$counts
```

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

• Use these for a  $\chi^2$  test

## X-squared

▶ Don't need to run hist first; can also use cut to discretize

- Better ways to do this
  - Loss of information from discretization
  - Lots of work just to use chisq.test()
- ► Try ks.test, "bootstrap" testing, "smooth tests of goodness of fit", . . .

### Summary

- Random number generation
- ▶ Distributions in R
- Parametric distributions are models
- Methods of fitting; moments, generalized moments, likelihood
- Methods of checking; visual comparisons, other statistics, tests, calibration