Lecture 2: Parameter Estimation

STA261 − Probability & Statistics II

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Outline

Introduction: Probabilistic Modelling in Science

Example: Emissions of Alpha Particles

Parameter Estimation

Method of Moments Estimation
Maximum Likelihood Estimation

Maximum Likelihood via Numerical Optimization

Motivating Example

The Newton-Raphson method



Radioactive Decay (Section 8.2 in the book)

 Radioactive material, emits α -particles

 period of observation

≪ half-life $(\Longrightarrow \text{emission rate} \approx \text{constant})$

• Rate, λ , classifies material

• We observe counts of α -particles

• What do the counts tell us about λ ?

• Have X - count for a 10 sec interval

Have 1207 non-overlapping intervals

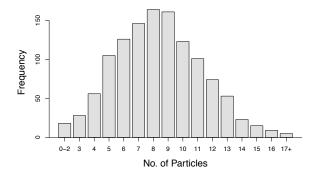
• Have X_i , i = 1, ..., 1207

	i
x	Observed Count
0,1,2	18
3	28
4	56
5	105
6	126
7	146
:	:
15	15
16	9
≥ 17	5

Table: Intervals were categorized by count

The data

```
> observed <- c(18, 28, 56, 105, 126, 146, 164, 161,
                123, 101, 74, 53, 23, 15, 9, 5)
> names <- c("0-2", paste(3:16), "17+")
>
> bp <- barplot(observed, names=names, axes=TRUE,
                xlab="No. of Particles", ylab="Frequency")
```



Randomness as a form of ignorance

- Clearly the number of particles emitted per time unit varies
- As science develops, the reasons for that may be uncovered
- For example, when a fair die is rolled, we say " $X \sim U\{1, \dots, 6\}$..."
 - Perhaps if we knew the initial position of the die, the release speed and angle etc., we could tell the result with certainty?
 - But that would be difficult...
- Turning to statistics/probability is oftentimes an admission of the limitations/inadequacy of a scientific theory
- "Essentially, all models are wrong, but some are useful." (George E.P. Box)
- With that in mind, we try to fit the best possible model to quantify the uncertainty with respect to all possible outcomes



Back to the α particles example

- Rate of emission is approximately constant
- No two particles can be emitted simultaneously
- This means that the Poisson distribution represents a reasonable model for the data:

$$X_1 \dots, X_n \stackrel{\text{i.i.d.}}{\sim} \text{Pois}(\lambda) \qquad (n = 1207)$$

- Note that the distribution of the number of particles emitted is completely determined by λ - the parameter of the distribution
- If we are to make any probabilistic statements about potential future outcomes (number of emitted particles), value must be provided for λ
 - or rather learned from the data!



Parameter estimation

Reminder

Any function of the sample is called a *statistic*.

Definition

Let X_1, \ldots, X_n be a random sample from some distribution, and let θ be a parameter of that distribution. Any statistic $U = U(X_1, \ldots, X_n)$ that is used to estimate θ , is called an *estimator* of θ .

- We usually denote an estimator of θ by $\widehat{\theta}$
 - In the particle emission example: $\hat{\lambda} = ?$
- In the next few weeks we will -
 - Introduce methods of estimation,
 - Discuss properties of estimators, and
 - Learn how to assess the performance of estimators



Method of Moments estimation

Definition

Let X_1, \ldots, X_n be a random sample from some distribution.

1. The kth moment of the distribution (if exists) is defined as

$$\mu_k = \mathbb{E}\left[X^k\right].$$

2. The kth sample moment is defined as

$$m_k = \frac{1}{n} \sum_{i=1}^n X_i^k.$$

• The method of moments estimator of $\boldsymbol{\theta} = (\theta_1, \dots, \theta_p)$ is the solution to the system

$$\begin{cases} \mu_1(\hat{\boldsymbol{\theta}}) = m_1 \\ \vdots \\ \mu_p(\hat{\boldsymbol{\theta}}) = m_p \end{cases}$$



Example: the normal distribution

Example

For $X_1, \ldots, X_n \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(\mu, \sigma^2)$, find the method of moments estimators of μ and σ .

Solution:

We need to solve the system

$$\begin{cases} \mu_1 = \mathbb{E}[X] = \overline{\mu} = m_1 = \frac{1}{n} \sum_{i=1}^n X_i = \overline{X}, \text{ and} \\ \mu_2 = \mathbb{E}[X^2] = \{\mathbb{E}[X]\}^2 + \text{Var}[X] = \underline{\mu}^2 + \underline{\sigma}^2 = m_2 = \frac{1}{n} \sum_{i=1}^n X_i^2, \end{cases}$$

for which the solution is

$$\mu=m_1=\overline{X}, \text{ and}$$

$$\sigma^2=m_2-m_1^2=\frac{1}{n}\sum_{i=1}^n X_i^2-\overline{X}^2.$$

then substitute estimator in place of true param



Example: the normal distribution (cont.)

Solution (cont.):

The Method of Moments estimators are then obtained by replacing each unknown parameter θ by $\widehat{\theta}$. In this case –

$$\begin{cases} \widehat{\mu} &= \overline{X}, \text{ and} \\ \\ \widehat{\sigma}^2 &= \frac{1}{n} \sum_{i=1}^n X_i^2 - \overline{X}^2. \end{cases}$$

* Note that

$$\widehat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n X_i^2 - \overline{X}^2 = \frac{1}{n} \sum_{i=1}^n X_i^2 - 2\overline{X}^2 + \overline{X}^2$$

$$= \frac{1}{n} \sum_{i=1}^n X_i^2 - \frac{2}{n} \overline{X} \sum_{i=1}^n X_i + \frac{1}{n} \sum_{i=1}^n \overline{X}^2 = \frac{1}{n} \sum_{i=1}^n \left(X_i^2 - 2X_i \overline{X} + \overline{X}^2 \right)$$

$$= \frac{1}{n} \sum_{i=1}^n (X_i - \overline{X})^2.$$



Example: the Gamma distribution

Example

For $X_1, \ldots, X_n \stackrel{\text{i.i.d.}}{\sim} \text{Gamma}(\alpha, \lambda)$ (with pdf $f(x) = \frac{\lambda^{\alpha}}{\Gamma(\alpha)} x^{\alpha - 1} e^{-\lambda x}, x \geq 0$), find the method of moments estimators of α and λ .

Solution:

We need to solve the system

$$\begin{cases} \mu_1 &= \mathbb{E}[X] = \frac{\alpha}{\lambda} = m_1 = \frac{1}{n} \sum_{i=1}^n X_i = \overline{X}, \text{ and} \\ \mu_2 &= \mathbb{E}[X^2] = \left\{ \mathbb{E}[X] \right\}^2 + \operatorname{Var}[X] = \left(\frac{\alpha}{\lambda}\right)^2 + \frac{\alpha}{\lambda^2} = m_2 = \frac{1}{n} \sum_{i=1}^n X_i^2, \end{cases}$$

Or, more compactly

$$\begin{cases} \frac{\alpha}{\lambda} &= \overline{X} \\ \frac{\alpha}{\lambda^2} &= \frac{1}{n} \sum_{i=1}^n X_i^2 - \overline{X}^2 = \frac{1}{n} \sum_{i=1}^n (X_i - \overline{X})^2 \end{cases}$$

remember the simplification here proved eariler



Example: the Gamma distribution (cont.)

Solution (cont.):

$$\begin{cases} \frac{\alpha}{\lambda} &= \overline{X} \\ \frac{\alpha}{\lambda^2} &= \frac{1}{n} \sum_{i=1}^{n} (X_i - \bar{X})^2 \end{cases}$$

Dividing the second equation by the first one, we obtain

$$\lambda = \frac{\overline{X}}{\frac{1}{n} \sum_{i=1}^{n} (X_i - \overline{X})^2} \text{ and } \alpha = \lambda \overline{X} = \frac{\overline{X}^2}{\frac{1}{n} \sum_{i=1}^{n} (X_i - \overline{X})^2},$$

and finally, the Method of Moments estimators are given by

$$\widehat{\lambda} = \frac{\overline{X}}{\frac{1}{n} \sum_{i=1}^{n} (X_i - \overline{X})^2} \left(= \frac{\widehat{\mu}}{\widehat{\sigma}^2} \right)$$
 and

$$\widehat{\alpha} = \frac{\overline{X}^2}{\frac{1}{2} \sum_{i=1}^{n} (X_i - \overline{X})^2} \quad \left(= \frac{\widehat{\mu}^2}{\widehat{\sigma}^2} \right).$$

can be computed from data, statistics



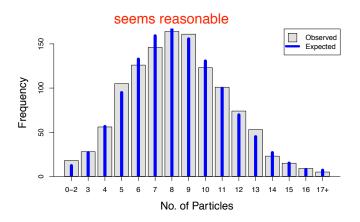
Back to the α particles example

- Here $X_1, \ldots, X_n \stackrel{\text{i.i.d.}}{\sim} \text{Pois}(\lambda)$ (n = 1207)
- Method of moments estimator: solve –

$$\mu_1 = \mathbb{E}[X] = \lambda = m_1 = \overline{X} \Longrightarrow \widehat{\lambda} = \overline{X}$$

- Our method of moments **estimator** is $\hat{\lambda} = \overline{X}$
- We are told that for our dataset $\hat{\lambda} = \overline{X} = 8.392$
 - Our method of moments **estimate** is $\hat{\lambda} = 8.392$
- Estimators are statistics (random variables); estimates are their evaluations (numbers)
- Is the Poisson model with $\hat{\lambda} = 8.392$ adequate for this kind of data?

Assessing the fit



$$\mathrm{Expected}_k = 1207 \times \mathrm{e}^{-\widehat{\lambda}} \frac{\widehat{\lambda}^k}{k!}$$

Consistency

Definition (Consistency)

Let $X_i, \ldots, X_n \sim f_\theta$ (a sample from a distribution depending on parameter θ). We say that $\widehat{\theta}_n = \widehat{\theta}_n(X_1, \dots, X_n)$ is a consistent estimator of θ if for any $\varepsilon > 0$

$$\lim_{n \to \infty} \mathbb{P}\left(|\widehat{\theta}_n - \theta| > \varepsilon\right) = 0.$$

- To be precise, the above property is called *consistency in probability*
- Sometimes we say that $\widehat{\theta}_n$ converges in probability to θ , or simply write $\widehat{\theta}_n \stackrel{\mathrm{P}}{\longrightarrow} \theta$
- In fact, we have all encountered one consistent estimator already... when we studied the Weak Law of Large Numbers (WLLN)!

i.e. $P(I \cdot bar\{X \mid n\} - \cdot mu \mid > \cdot epsilon) \cdot stackrel{p}{\cdot sim} 0$

Consistency of method of moments estimators

Reminder (WLLN)

Let X_i, \ldots, X_n be a random sample from some distribution with mean $\mathbb{E}[X]$. Then for any $\varepsilon > 0$

$$\lim_{n \to \infty} \mathbb{P}\left(\left| \frac{1}{n} \sum_{i=1}^{n} X_i - \mathbb{E}[X] \right| > \varepsilon \right) = 0.$$

- Thus $m_1 (= \overline{X})$ is a consistent estimator of the first moment $\mu_1 (= \mathbb{E}[X])$
- true regardless of distribution of X
 Replace X_i with X_i^k and $\mathbb{E}[X]$ with $\mathbb{E}[X^k]$ above, and you will learn that $m_k \xrightarrow{P} \mu_k$ for any k (as long as the latter exists)

Theorem

Let $\widehat{\theta}_n \stackrel{P}{\longrightarrow} \theta$ and $\widehat{\eta}_n \stackrel{P}{\longrightarrow} n$. Then

1.
$$\widehat{\theta}_n + \widehat{\eta}_n \stackrel{P}{\longrightarrow} \theta + \eta$$

2.
$$\widehat{\theta}_n \widehat{\eta}_n \stackrel{P}{\longrightarrow} \theta \eta$$

3.
$$q(\widehat{\theta}_n) \stackrel{P}{\longrightarrow} q(\theta)$$
 for any continuous $q: \mathbb{R} \to \mathbb{R}$



Consistency (cont.)

- The last Theorem is the reason why method of moments estimators are usually consistent
- Consider, for example

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (X_i - \overline{X})^2 = m_2 - m_1^2$$

we obtained for the normal distribution earlier

- $m_1 \xrightarrow{P} \mathbb{E}[X]$, hence $m_1^2 \xrightarrow{P} {\mathbb{E}[X]}^2$ (why?)
- $m_2 \xrightarrow{P} \mathbb{E}[X^2]$, therefore

by property 3 previous page

$$\widehat{\sigma}^2 = m_2 - m_1^2 \xrightarrow{P} \mathbb{E}[X^2] - \{\mathbb{E}[X]\}^2 = \sigma^2$$

Similarly,

$$S^{2} = \frac{1}{n-1} \sum_{i=1}^{n} (X_{i} - \overline{X})^{2} = \frac{n}{n-1} \cdot \widehat{\sigma}^{2} \xrightarrow{P} 1 \cdot \sigma^{2} = \sigma^{2}$$

sample variance is also consistent



Method of moments: concluding remarks

- Method of moments estimators are typically easy to derive
- Could lead to conflicting results (non-unique solutions) in the Poisson example we obtained $\hat{\lambda} = \overline{X}$, but note that

$$\mu_1 = \mathbb{E}[X] = \lambda = m_1,$$

 $\mu_2 = \mathbb{E}[X^2] = \text{Var}[X] + {\{\mathbb{E}[X]\}}^2 = \lambda + \lambda^2 = m_2,$

note here estimator derived from second order moments different from first

hence
$$\hat{\lambda} = m_2 - m_1^2 = \frac{1}{n} \sum_{i=1}^n X_i^2 - \overline{X}^2 = \hat{\sigma}^2$$
 is another method of moments

- estimator of λ
- Despite being consistent, they are often outperformed by other methods of estimation
- We may use them as initial values in iterative procedures when searching for Maximum Likelihood Estimators

Maximum Likelihood Estimation

Definition

Let $X_1 \ldots, X_n$ be continuous (discrete) random variables with joint pdf (pmf) $f(x_1,\ldots,x_n|\theta)$, where θ is a parameter. For a given vector of observations (x_1,\ldots,x_n) , the *likelihood* of θ is

$$\mathcal{L}(\theta) = f(x_1, \dots, x_n | \theta).$$

- In words: "how likely are we to observe such a sample for this particular value of θ ?"
- We are used to thinking of the joint pdf (pmf) as a function of randomly drawn X's with the parameters known and fixed
- Here the sample is observed and held fixed, while we let the (unknown) parameters vary
- Our goal is to choose among all possible values of θ , the one most likely to have produced the sample in hand

Example: Poisson distribution

- As before $X_1, \ldots, X_n \stackrel{\text{i.i.d.}}{\sim} \text{Pois}(\lambda)$
- $P(X_i = x_i | \lambda) = e^{-\lambda} \frac{\lambda^{x_i}}{x_i!}, x_i = 0, 1, 2, ..., i = 1, ..., n$
- The likelihood in this case is given by –

$$\mathcal{L}(\lambda) = P(x_1, \dots, x_n | \lambda) \xrightarrow{\text{ind}} \prod_{i=1}^n P(X_i = x_i | \lambda)$$
$$= \prod_{i=1}^n \frac{\lambda^{x_i} e^{-\lambda}}{x_i!} = \lambda^{\sum_{i=1}^n x_i} e^{-n\lambda} / \prod_{i=1}^n x_i!$$
$$\propto \lambda^{n\bar{x}} e^{-n\lambda}$$

Definition

The Maximum Likelihood Estimator (MLE) of θ is

$$\widehat{\boldsymbol{\theta}}_{\mathrm{MLE}} = \arg \max_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta})$$

(the value of θ that maximizes $\mathcal{L}(\theta)$).



Example: Poisson distribution (cont.)

$$\mathcal{L}(\lambda) \propto \lambda^{n\bar{x}} e^{-n\lambda}$$

- We wish to find $\widehat{\lambda}_{\text{MLE}} = \arg \max_{\lambda} \mathcal{L}(\lambda)$
- It is often more convenient to work with the log-likelihood function,

$$\ell(\lambda) := \log \mathcal{L}(\lambda) = n\bar{x} \log \lambda - n\lambda + \text{const}$$

- Turns products into sums
- Prevents computer underflow errors
- Because the logarithm is a monotonically increasing function

$$\arg\max_{\lambda}\ell(\lambda) = \arg\max_{\lambda}\mathcal{L}(\lambda)$$

justification why maximizing log likelihood still works



Example: Poisson distribution (cont.)

$$\ell(\lambda) = n\bar{x}\log\lambda - n\lambda + \text{const}$$

• Maximize $\ell(\lambda)$:

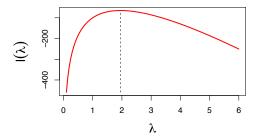
$$\frac{\partial \ell}{\partial \lambda} = \frac{n\bar{x}}{\lambda} - n = 0 \Longrightarrow \lambda = \bar{x}$$

- Hence $\widehat{\lambda}_{\text{MLE}} = \overline{X}$
- Verify maximum:

$$\left. \frac{\partial^2 \ell}{\partial \lambda^2} \right|_{\lambda = \bar{x}} = \left. - \frac{n\bar{x}}{\lambda^2} \right|_{\lambda = \bar{x}} = \left. - \frac{n}{\bar{x}} < 0 \right.$$

Poisson example: R simulation

```
lambda <- 2
n <- 100
x <- rpois(n, lambda) #sampling 100 random Poisson RVs
lambdaValues <- seq(.1, 6, by=.05)
xBar <- mean(x) #the MLE
loglike <- n*xBar*log(lambdaValues) - n*lambdaValues
plot(lambdaValues, loglike, type='1')
lines(c(xBar, xBar), c(min(loglike), max(loglike)), lty=2)
```





Example: MLEs for the normal distribution

Example

For $X_1, \ldots, X_n \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(\mu, \sigma^2)$, find the maximum likelihood estimators of μ and σ .

Solution:

The likelihood in this case is

$$\mathcal{L}(\mu, \sigma^2) = f(x_1, \dots, x_n | \mu, \sigma^2) \stackrel{\text{ind}}{=} \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i - \mu)^2}{2\sigma^2}}$$

$$\propto (\sigma^2)^{-n/2} \exp \left\{ -\frac{1}{2\sigma^2} \sum_{i=1}^n (x_i - \mu)^2 \right\},$$

and the log-likelihood is consequently

$$\ell(\mu, \sigma^2) = -\frac{n}{2} \log \sigma^2 - -\frac{1}{2\sigma^2} \sum_{i=1}^n (x_i - \mu)^2 + \text{const.}$$



MLEs for the normal distribution (cont.)

$$\ell(\mu, \sigma^2) = -\frac{n}{2}\log \sigma^2 - \frac{1}{2\sigma^2} \sum_{i=1}^n (x_i - \mu)^2 + \text{const.}$$

Now, solving

$$\frac{\partial \ell}{\partial \mu} = \frac{1}{\sigma^2} \sum_{i=1}^n (x_i - \mu) = 0 \Longrightarrow \sum_{i=1}^n x_i = n\mu \Longrightarrow \widehat{\mu} = \frac{1}{n} \sum_{i=1}^n x_i = \overline{X},$$

and

$$\frac{\partial \ell}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} \sum_{i=1}^{n} (x_i - \mu)^2 = 0$$

$$\Longrightarrow \widehat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \widehat{\mu})^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{X})^2.$$
note we substituted \mu = mean in

* Do not expect the MLEs to always coincide with the Method of Moments note its each individual data - mean estimators...



points(mu.hat, sigma.hat, cex=2.5, pch=18)

Normal example: R simulation

```
y <- c(200.3, 195.0, 192.4, 205.2, 190.1)
                                                                          Normal Likelihood vs. \mu and \sigma
n <- length(y)
mu.hat <- mean(v)
                                                               ß
sigma.hat \leftarrow sqrt((sd(y))^2*(n-1)/n)
                                                               9
muVec <- seq(190, 204, length = 150)
sigmaVec <- seq(3, 13, length = 150)
                                                           р
                                                               œ
LogLikeli <- function(mu, sigma)
        -n*log(sigma) - sum((y-mu)^2)/(2*sigma^2)
                                                               9
}
Z <- outer(muVec, sigmaVec,
     function(mu, sigma) mapply(LogLikeli, mu, sigma))
                                                                 190
                                                                       192
                                                                             194
                                                                                                200
                                                                                                      202
contour(muVec, sigmaVec, exp(Z), nlevel=20)
```



Parameter estimation for muon decay

Example

Denote by Θ the angle at which electrons are released in a muon decay, and let $X = \cos \Theta$. If we assume that X follows a distribution with pdf

$$f(x\big|\alpha) = \frac{1+\alpha x}{2}, \ -1 \le x \le 1, \ -1 \le \alpha \le 1,$$

find both method of moments and maximum likelihood estimators for α , based on a random sample X_1, \ldots, X_n .

Solution:

• First note that note in this case pdf is continuous

$$\mathbb{E}[X] = \int x f(x|\alpha) dx = \frac{1}{2} \int_{-1}^{1} (x + \alpha x^2) dx = \frac{\alpha}{3},$$

thus the method of moments estimator of α can be derived by solving

$$\mu_1 = \mathbb{E}[X] = \frac{\alpha}{3} = m_1 = \overline{X} \Longrightarrow \widehat{\alpha} = 3\overline{X}$$



Muon decay example (cont.)

- Onto finding the MLE of α
- Write the likelihood:

$$\mathcal{L}(\alpha) = f(x_1, \dots, x_n | \alpha) = \prod_{i=1}^n f(x_i | \alpha) = \frac{1}{2^n} \prod_{i=1}^n (1 + \alpha x_i)$$

• On the logarithmic scale:

$$\ell(\alpha) = -n\log 2 + \sum_{i=1}^{n} \log(1 + \alpha x_i)$$

• To find the $\widehat{\alpha}_{\mathrm{MLE}}$ we need to solve

$$\frac{\partial \ell}{\partial \alpha} = \sum_{i=1}^{n} \frac{x_i}{1 + \alpha x_i} = 0$$



no closed form so iterative method

The Newton-Raphson method

- To find the MLE of θ we need to solve $\ell'(\theta)\Big|_{\theta=\widehat{\theta}}=0$
- For θ_0 in the proximity of $\widehat{\theta}$,

$$\ell'(\hat{\theta}) \approx \ell'(\theta_0) + \ell''(\theta_0)(\hat{\theta} - \theta_0)$$
 (first order Taylor expansion about θ_0) condition which derives the mle estimator

• However, $\ell'(\hat{\theta}) = 0$ (why?), hence

$$\ell'(\theta_0) + \ell''(\theta_0)(\hat{\theta} - \theta_0) \approx 0,$$

or, alternatively

$$\widehat{\theta} \approx \theta_0 - \frac{\ell'(\theta_0)}{\ell''(\theta_0)}$$

This is the Newton-Raphson method -

$$\widehat{\theta}_{\text{new}} = \widehat{\theta}_{\text{old}} - \frac{\ell'(\widehat{\theta}_{\text{old}})}{\ell''(\widehat{\theta}_{\text{old}})} \text{ (iterate until convergence)}$$



Back to the muon decay example

•
$$\ell'(\alpha) = \sum_{i=1}^{n} \frac{x_i}{1 + \alpha x_i}$$

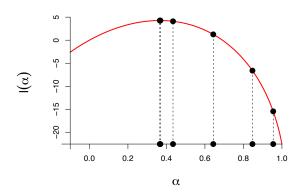
•
$$\ell''(\alpha) = -\sum_{i=1}^{n} \frac{x_i^2}{(1 + \alpha x_i)^2}$$

•
$$\widehat{\alpha}_{\text{new}} = \widehat{\alpha}_{\text{old}} - \frac{\ell'(\widehat{\alpha}_{\text{old}})}{\ell''(\widehat{\alpha}_{\text{old}})}$$

 alpha <- runif(1) #random initial value tolerance <- 5e-16 #largest difference between successive alphas delta <- 1 LogLikeOld <- sum(log(1 + alpha*x)) #log-likelihood at initial alpha while(delta > tolerance){ 1Prime <- sum(x/(1 + alpha*x)) #first derivative 12Prime <- -sum(x^2/(1 + alpha*x)^2) #second derivative alpha <- alpha - 1Prime/12Prime #Newton-Raphson update LogLike <- sum(log(1 + alpha*x)) #log-likelihood at new alpha delta <- abs(LogLike - LogLikeOld) #difference LogLikeOld <- LogLike }



Muon decay example (cont.)



- > alpha #maximum likelihood estimate
- [1] 0.3657926
- > (alphaHatMME <- 3*mean(x)) #method of moments estimate
- [1] 0.3444427