

# Maximum Likelihood

STA2101 Fall 2019

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# Maximum Likelihood

$$X_1, \dots, X_n \stackrel{i.i.d.}{\sim} F_\theta, \theta \in \Theta$$

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

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

# Close your eyes and differentiate?

Let  $X_1, \dots, X_n$  be a random sample from a Gamma distribution with parameters  $\alpha > 0$  and  $\beta > 0$

$$f(x; \alpha, \beta) = \frac{1}{\beta^\alpha \Gamma(\alpha)} e^{-x/\beta} x^{\alpha-1}$$

$$\Theta = \{(\alpha, \beta) : \alpha > 0, \beta > 0\}$$

# Simulate Some Data: True $\alpha=2$ , $\beta=3$

```
> set.seed(3201); alpha=2; beta=3
> D <- round(rgamma(50,shape=alpha, scale=beta),2); D
 [1] 20.87 13.74  5.13  2.76  4.73  2.66 11.74  0.75 22.07 10.49  7.26  5.82 13.08
[14]  1.79  4.57  1.40  1.13  6.84  3.21  0.38 11.24  1.72  4.69  1.96  7.87  8.49
[27]  5.31  3.40  5.24  1.64  7.17  9.60  6.97 10.87  5.23  5.53 15.80  6.40 11.25
[40]  4.91 12.05  5.44 12.62  1.81  2.70  3.03  4.09 12.29  3.23 10.94
> mean(D); alpha*beta
[1] 6.8782
[1] 6
> var(D); alpha*beta^2
[1] 24.90303
[1] 18
```

Alternatives for getting the data into D might be

D = scan("Gamma.data") -- Can put entire URL

D = c(20.87, 13.74, ..., 10.94)

# Log Likelihood

$$\begin{aligned}\ell(\alpha, \beta) &= \ln \prod_{i=1}^n \frac{1}{\beta^\alpha \Gamma(\alpha)} e^{-x_i/\beta} x_i^{\alpha-1} \\ &= \ln \left[ \beta^{-n\alpha} \Gamma(\alpha)^{-n} \exp\left(-\frac{1}{\beta} \sum_{i=1}^n x_i\right) \left(\prod_{i=1}^n x_i\right)^{\alpha-1} \right] \\ &= -n\alpha \ln \beta - n \ln \Gamma(\alpha) - \frac{1}{\beta} \sum_{i=1}^n x_i + (\alpha - 1) \sum_{i=1}^n \ln x_i\end{aligned}$$

# R function for the minus log likelihood

$$\ell(\alpha, \beta) = -n\alpha \ln \beta - n \ln \Gamma(\alpha) - \frac{1}{\beta} \sum_{i=1}^n x_i + (\alpha - 1) \sum_{i=1}^n \ln x_i$$

```
> # Gamma minus log likelihood: alpha=a, beta=b
> gmll <- function(theta,datta)
+   {
+     a <- theta[1]; b <- theta[2]
+     n <- length(datta); sumd <- sum(datta)
+     sumlogd <- sum(log(datta))
+     gmll <- n*a*log(b) + n*lgamma(a) + sumd/b - (a-1)*sumlogd
+     gmll
+   } # End function gmll
```

# Where should the numerical search start?

- How about Method of Moments estimates?
- $E(X) = \alpha\beta$ ,  $\text{Var}(X) = \alpha\beta^2$
- Solve for  $\alpha$  and  $\beta$ , replace population moments by sample moments and put a  $\sim$  above the parameters.

$$\tilde{\alpha} = \frac{\overline{X^2}}{S^2} \quad \text{and} \quad \tilde{\beta} = \frac{S^2}{\overline{X}}$$

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```
> momalpha <- mean(D)^2/var(D); momalpha  
[1] 1.899754  
> mombeta <- var(D)/mean(D); mombeta  
[1] 3.620574
```



```
> gammasearch = nlm(gmll,c(momalpha,mombeta),hessian=T,datta=D); gammasearch
```

```
$minimum
```

```
[1] 142.0316
```

$$-\ell(\hat{\alpha}, \hat{\beta})$$

```
$estimate
```

```
[1] 1.805930 3.808674
```

$$\hat{\alpha} = 1.805930 \quad \hat{\beta} = 3.808674$$

```
$gradient
```

```
[1] 2.847002e-05 9.133932e-06
```

$$\left( -\frac{\partial \ell}{\partial \alpha}, -\frac{\partial \ell}{\partial \beta} \right)^\top$$

```
$hessian
```

```
      [,1]      [,2]  
[1,] 36.68932 13.127271  
[2,] 13.12727  6.222282
```

$$\mathbf{H} = \left[ \frac{\partial^2(-\ell)}{\partial \theta_i \partial \theta_j} \right]$$

```
$code
```

```
[1] 1
```

```
$iterations
```

```
[1] 6
```

```
> eigen(gammasearch$hessian)$values
```

```
[1] 41.565137  1.346466
```

$$\mathbf{H} = \left[ \frac{\partial^2(-\ell)}{\partial\theta_i\partial\theta_j} \right]$$

If the second derivatives are continuous,  $\mathbf{H}$  is symmetric.

If the gradient is zero at a point and  $|\mathbf{H}| \neq 0$ ,

If  $\mathbf{H}$  is positive definite, local minimum

If  $\mathbf{H}$  is negative definite, local maximum

If  $\mathbf{H}$  has both positive and negative eigenvalues, saddle point

# A slicker way to define the minus log likelihood function

```
> gml12 <- function(theta,datta)
+   { gml12 <- -sum(dgamma(datta,shape=theta[1],scale=theta[2],log=T))
+     gml12
+   } # End of gml12

> nlm(gml12,c(momalpha,mombeta),datta=D)
$minimum
[1] 142.0316

$estimate
[1] 1.805930 3.808674

$gradient
[1] 2.847002e-05 9.133932e-06

$code
[1] 1

$iterations
[1] 6
```

# Likelihood Ratio Tests

$$X_1, \dots, X_n \stackrel{i.i.d.}{\sim} F_\theta, \theta \in \Theta,$$
$$H_0 : \theta \in \Theta_0 \text{ v.s. } H_A : \theta \in \Theta \cap \Theta_0^c,$$

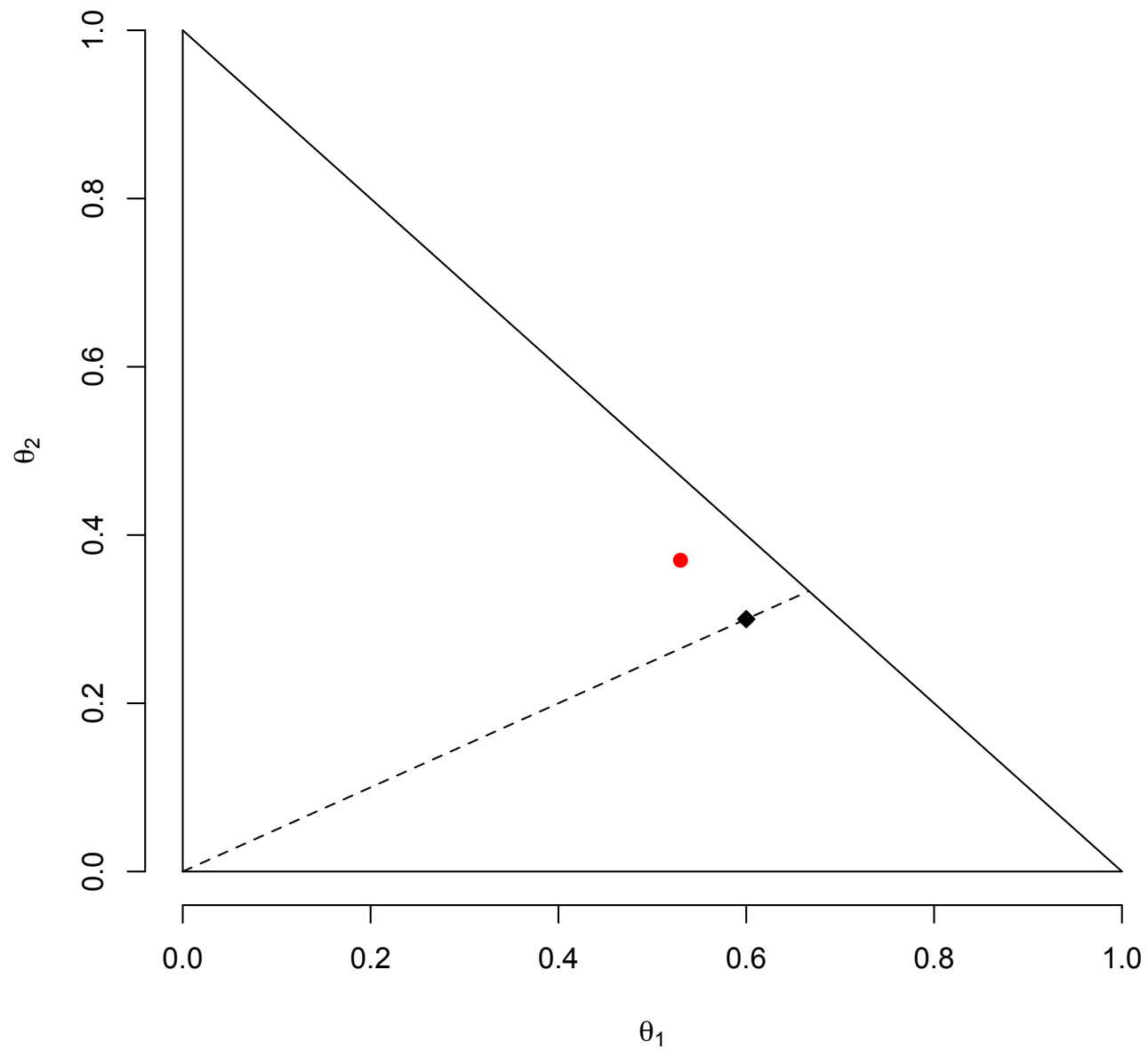
$$G^2 = -2 \log \left( \frac{\max_{\theta \in \Theta_0} L(\theta)}{\max_{\theta \in \Theta} L(\theta)} \right)$$

Under  $H_0$ ,  $G^2$  has an approximate chi-square distribution for large  $N$ . Degrees of freedom = number of (non-redundant, linear) equalities specified by  $H_0$ . Reject when  $G^2$  is large.

# Example: Multinomial with 3 categories

- Parameter space is 2-dimensional
- Unrestricted MLE is  $(P_1, P_2)$ : Sample proportions.
- $H_0: \theta_1 = 2\theta_2$

# Parameter space and restricted parameter space



# R code for the record

```
# Plotting jobs parameter space with R
# Including MLE and restricted MLE
theta1 = seq(from=0,to=1,by=0.05); theta2=theta1
plot(theta1,theta2,pch=' ', frame.plot=F,
      xlab=expression(theta[1]), ylab=expression(theta[2]))
# Draw boundaries of parameter space
xloc1 = c(0,0); yloc1 = c(0,1); lines(xloc1,yloc1,lty=1)
xloc2 = c(0,1); yloc2 = c(0,0); lines(xloc2,yloc2,lty=1)
xloc3 = c(0,1); yloc3 = c(1,0); lines(xloc3,yloc3,lty=1)
# Restricted parameter space is a line segment
xloc4 = c(0,2/3); yloc4 = c(0,1/3); lines(xloc4,yloc4,lty=2)

points(0.53,0.37, pch=19, col = "red1") # Unrestricted MLE
points(0.60,0.30, pch=23, bg="black") # Restricted MLE
```

# Degrees of Freedom

Express  $H_0$  as a set of linear combinations of the parameters, set equal to constants (usually zeros).

Degrees of freedom = number of *non-redundant* linear combinations (meaning linearly independent).

Suppose  $\boldsymbol{\theta} = (\theta_1, \dots, \theta_7)$ , with

$$H_0 : \theta_1 = \theta_2, \theta_6 = \theta_7, \frac{1}{3} (\theta_1 + \theta_2 + \theta_3) = \frac{1}{3} (\theta_4 + \theta_5 + \theta_6)$$

df=3 (count the = signs)



# Can write Null Hypothesis in Matrix Form as $H_0: \mathbf{L}\boldsymbol{\theta} = \mathbf{h}$

$$H_0 : \theta_1 = \theta_2, \theta_6 = \theta_7, \frac{1}{3} (\theta_1 + \theta_2 + \theta_3) = \frac{1}{3} (\theta_4 + \theta_5 + \theta_6)$$

$$\begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 & 0 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \\ \theta_5 \\ \theta_6 \\ \theta_7 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Rows are linearly independent, so  $df$  = number of rows.

# Gamma Example: $H_0: \alpha = \beta$

$$\begin{aligned} G^2 &= -2 \log \left( \frac{\max_{\theta \in \Theta_0} L(\theta)}{\max_{\theta \in \Theta} L(\theta)} \right) \\ &= 2 \left( -\ell(\hat{\theta}_0) - [-\ell(\hat{\theta})] \right) \end{aligned}$$

Already have  $-\ell(\hat{\theta}) = 142.0316$

Could re-write the function imposing constraints: Not recommended

# Make a wrapper function

```
> gml12 <- function(theta,datta)
+   { gml12 <- -sum(dgamma(datta,shape=theta[1],scale=theta[2],log=T))
+     gml12
+   } # End of gml12
```

```
> gml1H0 <- function(theta,datta) # Theta is a scalar this time
+   { gml1H0 <- gml12(c(theta,theta),datta)
+     gml1H0
+   } # End of gml1H0
> H0start <- sqrt(mean(D)) # Because  $E(X) = \alpha \beta$ 
> H0start
[1] 2.622632
```

```
> nlm(gmllH0,H0start,datta=D)
```

```
$minimum
```

```
[1] 144.1704
```

```
$estimate
```

```
[1] 2.562369
```

```
$gradient
```

```
[1] 5.545982e-08
```

```
$code
```

```
[1] 1
```

```
$iterations
```

```
[1] 3
```

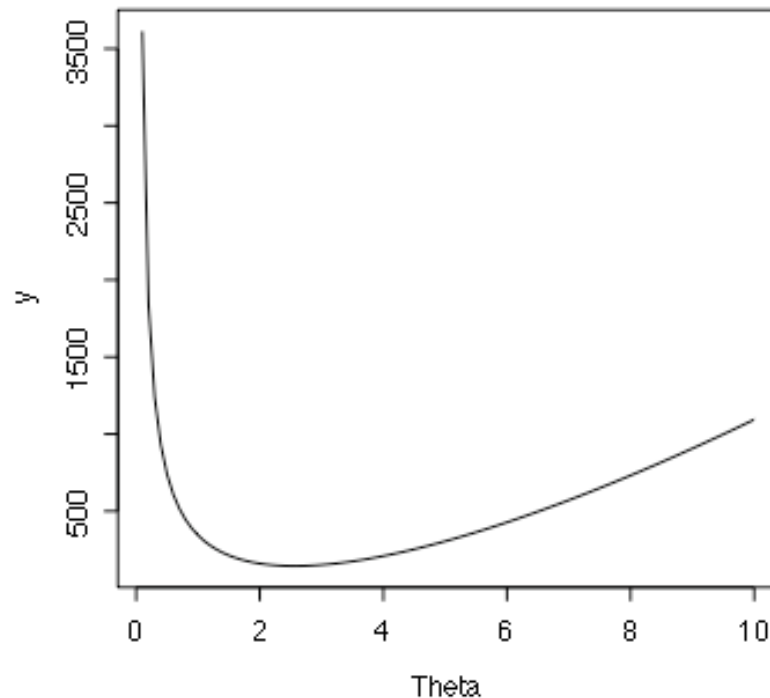
```
Warning messages:
```

```
1: NaNs produced in: dgamma(x, shape, scale, log)
```

```
2: NA/Inf replaced by maximum positive value
```

# It's probably okay, but plot -LL

```
> # It's probably okay, but plot  
> Theta = seq(from=0.1,to=10,by=0.1)  
> y = Theta-Theta  
> for(i in 1:length(Theta)) y[i] = gml1H0(Theta[i],D)  
> plot(Theta,y,type='l')
```



Test  $H_0: \alpha = \beta$

```
> G2 = 2 * (144.1704 - 142.0316); G2
```

```
[1] 4.2776
```

```
> 1 - pchisq(G2, df=1)
```

```
[1] 0.03861784
```

# The actual Theorem (Wilks, 1934)

- There are  $r+p$  parameters
- Null hypothesis says that the first  $r$  parameters equal specified constants.
- Then under some regularity conditions,  $G^2$  converges in distribution to chi-squared with  $r$  df if  $H_0$  is true.
- Can justify tests of *linear* null hypotheses by a re-parameterization using the invariance principle.

# How it works

- The invariance principle of maximum likelihood estimation says that the MLE of a function is that function of the MLE. Like

$$\hat{\sigma} = \sqrt{\widehat{\sigma^2}}$$

- Meaning is particularly clear when the function is one-to-one.
- Write  $H_0: \mathbf{L}\boldsymbol{\theta} = \mathbf{h}$ , where  $\mathbf{L}$  is  $r \times (r+p)$  and rows of  $\mathbf{L}$  are linearly independent.
- Can always find an additional  $p$  vectors that, together with the rows of  $\mathbf{L}$ , span  $\mathbb{R}^{r+p}$
- This defines a (linear) 1-to-1 re-parameterization, and Wilks' theorem applies directly.



# Gamma Example $H_0: \alpha = \beta$

Re-parameterize: Let

$$\theta_1 = \alpha - \beta$$

$$\theta_2 = \beta$$

The re-parameterization is one-to-one because

$$\alpha = \theta_1 + \theta_2$$

$$\beta = \theta_2$$

Invariance says  $\hat{\theta}_1 = \hat{\alpha} - \hat{\beta}$  and  $\hat{\theta}_2 = \hat{\beta}$

$$H_0 : \theta_1 = 0$$

# Can Work for Non-linear Null Hypotheses Too

$$X_1, \dots, X_n \stackrel{i.i.d.}{\sim} N(\mu, \sigma^2)$$

$$H_0 : \mu^2 = \sigma^2$$

Re-parameterize: Let

$$\theta_1 = \mu^2 - \sigma^2$$

$$\theta_2 = \mu$$

The re-parameterization is one-to-one because

$$\mu = \theta_2$$

$$\sigma^2 = \theta_2^2 - \theta_1$$

Invariance says  $\hat{\theta}_1 = \hat{\mu}^2 - \hat{\sigma}^2$  and  $\hat{\theta}_2 = \hat{\mu}$

$$H_0 : \theta_1 = 0$$

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