PLSC 504 – Fall 2020
Likelihood, Optimization, etc.

August 26, 2020

Welcome!

- "Proseminar" in methods
- The instruction mode is synchronous remote, via Zoom, at: (https://psu.zoom.us/j/95348749707)
- Texts: Various (see the syllabus)
- All course materials: https://github.com/PrisonRodeo/PLSC504-2020-git
- Preceptor: Brandon Bolte (not this one)
- Software: R > Stata
- Grading: Ten homework assignments (@ 50 points), plus a final project (500 points)
- Contact me: zorn@psu.edu, or text (803) 553-4077

A Very Simple Model

$$Y \sim N(\mu, \sigma^2)$$

$$\begin{aligned} \mathsf{E}(Y) &= \mu \\ \mathsf{Var}(Y) &= \sigma^2 \end{aligned}$$

Some Data

$$
\begin{aligned}
Y &= 64 \\
&\quad 63 \\
&\quad 59 \\
&\quad 71 \\
&\quad 68
\end{aligned}
$$

$$\Pr(Y_i = y_i) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(Y_i - \mu)^2}{2\sigma^2}\right]$$

So

$$\begin{aligned}
\Pr(Y_1 = 64) &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(64 - \mu)^2}{2\sigma^2}\right] \\
\Pr(Y_2 = 63) &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(63 - \mu)^2}{2\sigma^2}\right] \\
&\ldots
\end{aligned}$$

$$\Pr(A, B | \Pr(A) \perp \Pr(B)) = \Pr(A) \times \Pr(B)$$

So:

$$\begin{aligned} \Pr(Y_1 = 64, Y_2 = 63) &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(64-\mu)^2}{2\sigma^2}\right] \times \\ &\quad \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(63-\mu)^2}{2\sigma^2}\right] \end{aligned}$$

More Generally...

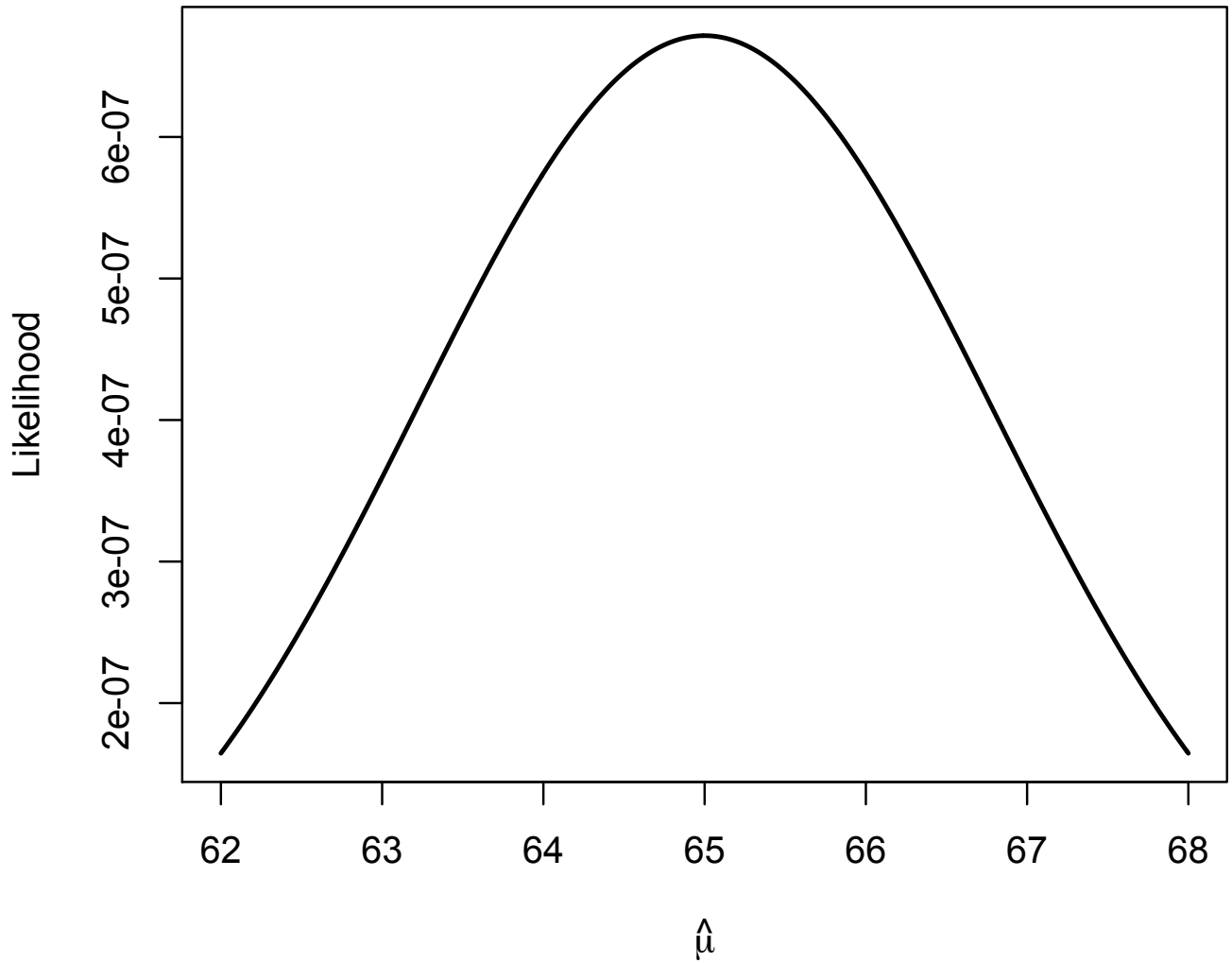
$$\begin{aligned}
\Pr(Y_i = y_i \ \forall \ i) &\equiv L(Y|\mu, \sigma^2) \\
&= \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(y_i - \mu)^2}{2\sigma^2}\right]
\end{aligned}$$

$$L(\hat{\mu}, \hat{\sigma}^2 | Y) \propto \Pr(Y | \hat{\mu}, \hat{\sigma}^2)$$

For $\hat{\mu} = 68$, $\hat{\sigma} = 4$:

$$\begin{aligned} L &= \frac{1}{\sqrt{2\pi 16}} \exp\left[-\frac{(64-68)^2}{32}\right] \times \\ &\quad \frac{1}{\sqrt{2\pi 16}} \exp\left[-\frac{(63-68)^2}{32}\right] \times \\ &\quad \frac{1}{\sqrt{2\pi 16}} \exp\left[-\frac{(59-68)^2}{32}\right] \times \ldots \\ &= \text{some reeeeeally small number...} \end{aligned}$$

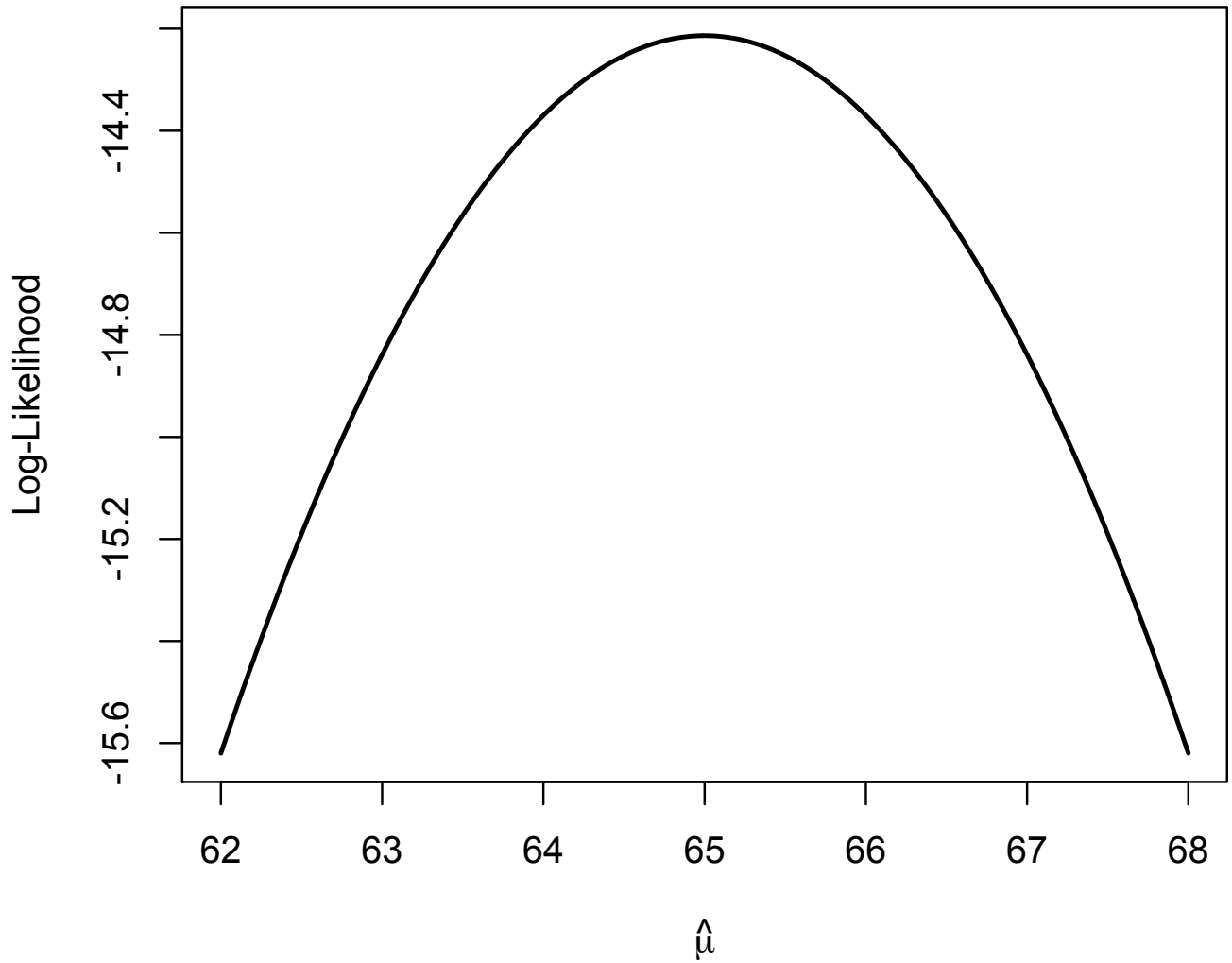
What a Likelihood Looks Like



Log-Likelihood

$$
\begin{aligned}
\ln L(\hat{\mu}, \hat{\sigma}^2 | Y) &= \ln \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(Y_i - \mu)^2}{2\sigma^2} \right] \\
&= \sum_{i=1}^{N} \ln \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(Y_i - \mu)^2}{2\sigma^2} \right] \right\} \\
&= -\frac{N}{2} \ln(2\pi) - \left[\sum_{i=1}^{N} \frac{1}{2} \ln\, \sigma^2 + \frac{1}{2\sigma^2} (Y_i - \mu)^2 \right]
\end{aligned}
$$

What a Log-Likelihood Looks Like



The "Maximum" Part

For $L = f(Y, \theta)$,

- Calculate $\frac{\partial \ln L}{\partial \theta}$,
- Set $\frac{\partial \ln L}{\partial \theta} = 0$, solve for $\hat{\theta}$,
- Calculate $\frac{\partial^2 \ln L}{\partial \theta^2}$,
- Verify $\frac{\partial^2 \ln L}{\partial \theta^2} < 0$.

Example: Normal Y

$$\ln L(\hat{\mu}, \hat{\sigma}^2 | Y) = -\frac{N}{2} \ln(2\pi) - \left[\sum_{i=1}^{N} \frac{1}{2} \ln \sigma^2 + \frac{1}{2\sigma^2} (Y_i - \mu)^2 \right]$$

$$\begin{aligned} \frac{\partial \ln L}{\partial \mu} &= \frac{1}{\sigma^2} \sum_{i=1}^{N} (Y_i - \mu) \\ \frac{\partial \ln L}{\partial \sigma^2} &= \frac{-N}{2\sigma^2} + \frac{1}{2} \sigma^4 \sum_{i=1}^{N} (Y_i - \mu)^2 \end{aligned}$$

Example: Normal Y (continued)

$\longrightarrow$

$$\hat{\mu} = \frac{1}{N}\sum_{i=1}^{N} Y_i$$

$$\hat{\sigma}^2 = \frac{1}{N}\sum_{i=1}^{N}(Y_i - \bar{Y})^2$$

Example: Linear Regression

$$\begin{aligned} \mathsf{E}(Y) \equiv \mu &= \beta_0 + \beta_1 X_i \\ \mathsf{Var}(Y) &= \sigma^2 \end{aligned}$$

$$L(\beta_0, \beta_1, \sigma^2 | Y) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(Y_i - \beta_0 - \beta_1 X_i)^2}{2\sigma^2} \right]$$

Linear Regression (continued)

$$\begin{aligned}
\ln L(\beta_0, \beta_1, \sigma^2 | Y) &= \ln \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(Y_i - \beta_0 - \beta_1 X_i)^2}{2\sigma^2} \right] \\
&= -\frac{N}{2} \ln(2\pi) - \sum_{i=1}^{N} \left[\frac{1}{2} \ln \sigma^2 + \frac{1}{2\sigma^2} (Y_i - \beta_0 - \beta_1 X_i)^2 \right]
\end{aligned}$$

Kernel:

$$-\sum_{i=1}^{N} \left[\frac{1}{2} \ln \sigma^2 + \frac{1}{2\sigma^2} (\underbrace{Y_i - \beta_0 - \beta_1 X_i}_{\hat{u}_i})^2 \right]$$

MLE in General

$$\Pr(Y) = f(\mathbf{X}, \theta)$$

$$L = \prod_{i=1}^{N} f(Y_i|\mathbf{X}_i, \theta)$$

$$\ln L = \sum_{i=1}^{N} \ln f(Y_i|\mathbf{X}_i, \theta)$$

$$\ln L(\hat{\theta}|Y, \mathbf{X}) = \max_{\theta} \{\ln L(\theta|Y, \mathbf{X})\}$$

$$\mathbf{g}(\hat{\theta}) = \frac{\partial \ln L(\hat{\theta})}{\partial \hat{\theta}}$$

Taylor series:

$$\frac{\partial \ln L}{\partial \hat{\theta}} \approx \frac{\partial \ln L}{\partial \theta} + \frac{\partial^2 \ln L}{\partial \theta^2}(\hat{\theta} - \theta)$$

$$\begin{aligned} \hat{\theta} - \theta &= \left(-\frac{\partial^2 \ln L}{\partial \theta^2}\right)^{-1} \frac{\partial \ln L}{\partial \theta} \\ &= -\mathbf{H}(\theta)^{-1}\mathbf{g}(\theta) \end{aligned}$$

Need

$$\text{plim}(\hat{\theta} - \theta) = 0$$

So:

- *Assume* $\mathbf{H}(\theta) \xrightarrow{a} \mathbf{A} < \infty$
- *Show* $\text{E}[\mathbf{g}(\theta)] \to \mathbf{0}$ as $N \to \infty$

Consistency (continued)

$$
\begin{aligned}
\mathsf{E}[\mathbf{g}(\theta)] &= \frac{1}{N}\,\mathsf{E}\left(\frac{\partial \ln L_1}{\partial \theta} + \frac{\partial \ln L_2}{\partial \theta} + \ldots + \frac{\partial \ln L_N}{\partial \theta}\right) \\
&= \frac{1}{N}\left[\mathsf{E}\left(\frac{\partial \ln L_1}{\partial \theta}\right) + \mathsf{E}\left(\frac{\partial \ln L_2}{\partial \theta}\right) + \ldots\right] \\
&\stackrel{a}{=} \mathbf{0}
\end{aligned}
$$

Cramer-Rao say:

$$\mathrm{Var}(\hat{\theta}) \geq \left[-\mathrm{E}\left(\frac{\partial^2 \ln L(\theta)}{\partial \theta^2} \right) \right]^{-1}$$

Efficiency, continued

$$\begin{aligned}
\mathrm{Var}(\hat{\theta}) &= \mathrm{E}[(\hat{\theta}-\theta)(\hat{\theta}-\theta)'] \\
&= \mathrm{E}\left[\left(-\frac{\partial^2 \ln L}{\partial\theta^2}\right)^{-1} \frac{\partial \ln L}{\partial\theta}\frac{\partial \ln L'}{\partial\theta}\left(-\frac{\partial^2 \ln L}{\partial\theta^2}\right)^{-1}\right]
\end{aligned}$$

For MLE:

$$\mathrm{E}\left[\frac{\partial \ln L}{\partial\theta}\frac{\partial \ln L'}{\partial\theta}\right] = \mathrm{E}\left[\frac{\partial^2 \ln L}{\partial\theta^2}\right]$$

So,

$$\begin{aligned}
\mathrm{Var}(\hat{\theta}) &= \left[-\mathrm{E}\left(\frac{\partial^2 \ln L}{\partial\theta^2}\right)\right]^{-1} \\
&= [\mathbf{I}(\theta)]^{-1}
\end{aligned}$$

By LLN:

$$\frac{\hat{\theta} - \theta}{\sqrt{\mathbf{I}(\theta)^{-1}}} \sim N(\mathbf{0}, \mathbf{1})$$

Or:

$$\hat{\theta} \sim N(\theta, \mathbf{I}(\theta)^{-1})$$

Invariance: Parameters

For

$$\gamma = h(\theta)$$

$$\hat{\gamma}_{ML} = h(\hat{\theta}_{ML})$$

Suppose

$$\phi^2 = 1/\sigma^2$$

so that

$$Y \sim N(\mu, \phi^2).$$

Then:

$$\ln L(\hat{\mu}, \hat{\phi}^2) = -\left[\sum_{i=1}^{N} \frac{1}{2} \ln \phi^2 - \frac{1}{2\phi^2}(Y_i - \mu)^2\right]$$

and:

$$\frac{\partial \ln L}{\partial \phi^2} = \frac{-N}{2\phi^2} + \frac{1}{2}\phi^4 \sum_{i=1}^{N}(Y_i - \mu)^2$$

and:

$$\begin{aligned} \hat{\phi}^2 &= \frac{N}{\sum_{i=1}^{N}(Y_i - \bar{Y})^2} \\ &= \frac{1}{\hat{\sigma}^2} \end{aligned}$$

Summary

MLEs:

- Maximize $L(\theta|Y, \mathbf{X})$
- Are consistent in N
- Are asymptotically efficient
- Are asymptotically Normal
- Are invariant to (injective) transformations and varying sampling methods

Optimization

The Basic Problem

Find

$$\max_{\hat{\boldsymbol{\beta}} \in \mathbb{R}^k} \ln L(\hat{\boldsymbol{\beta}} | Y, \mathbf{X})$$

Unconstrained optimization problem...

The Intuition

- Start with $\hat{\boldsymbol{\beta}}_{\mathbf{0}}$
- Adjust:

$$\hat{\boldsymbol{\beta}}_{\mathbf{1}} = \hat{\boldsymbol{\beta}}_{\mathbf{0}} + \mathbf{A}_{\mathbf{0}}$$

- Repeat.

More Specifically...

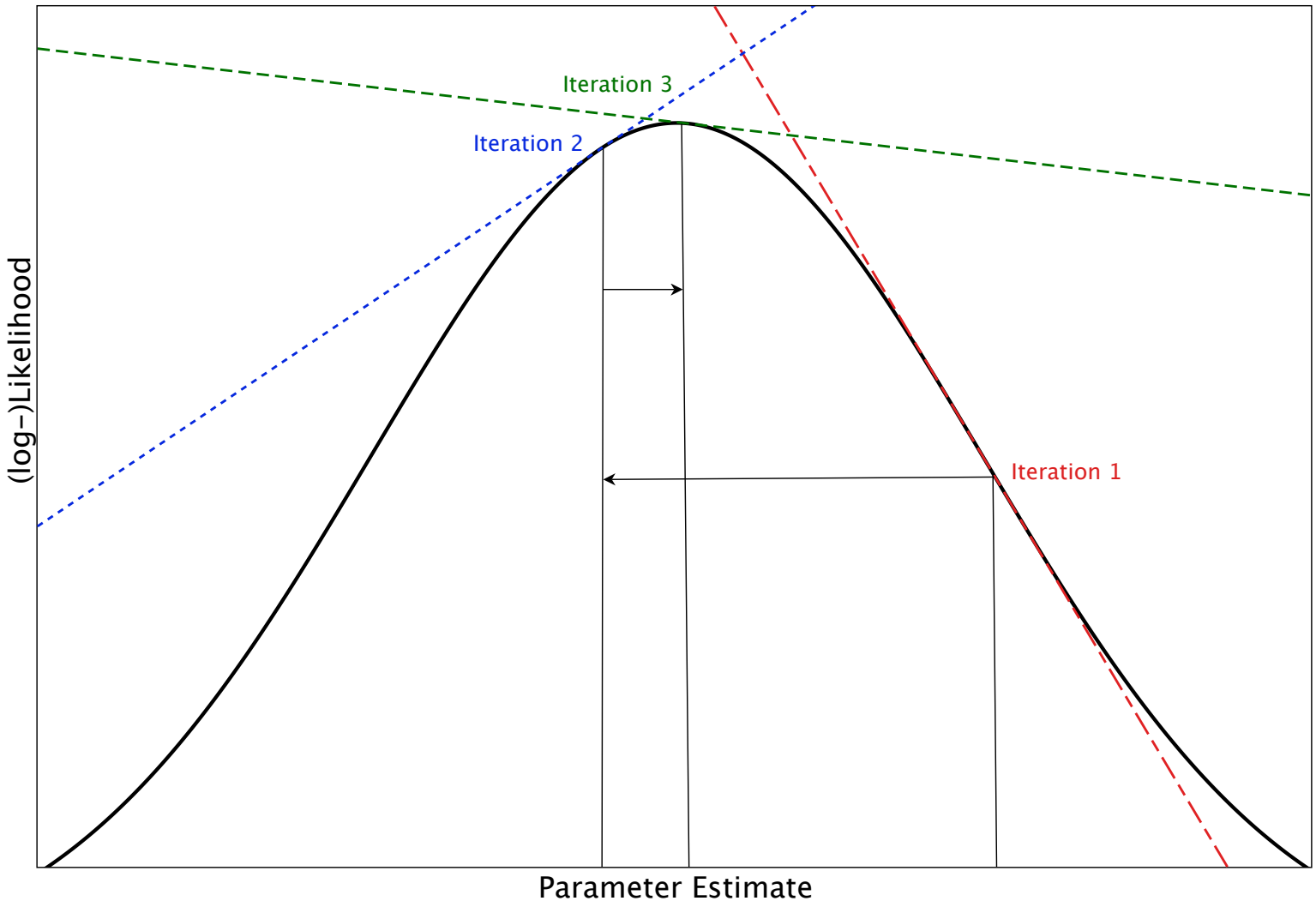
$$\hat{\boldsymbol{\beta}}_{\ell} = \hat{\boldsymbol{\beta}}_{\ell-\mathbf{1}} + \mathbf{A}_{\ell-\mathbf{1}}$$

$$\hat{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}}_{\ell} \ni \hat{\boldsymbol{\beta}}_{\ell} - \hat{\boldsymbol{\beta}}_{\ell-1} (\equiv \mathbf{A}_{\ell}) < \tau$$

What's **A**?

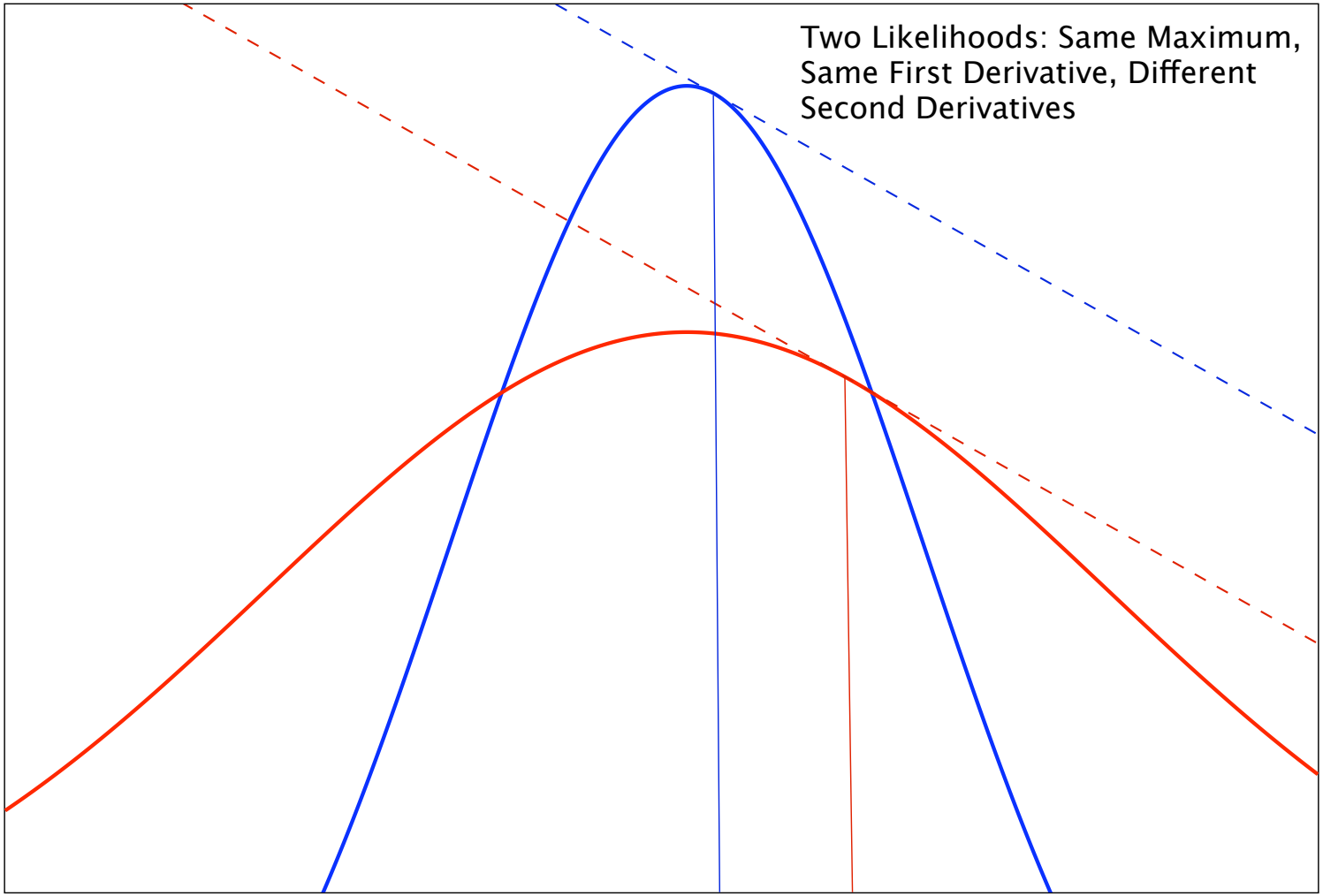
$$\mathbf{A} = f[\mathbf{g}(\hat{\boldsymbol{\beta}})]$$

- $\mathbf{g}(\hat{\boldsymbol{\beta}}) =$ "directionality" of change
  - $\mathbf{g}(\hat{\beta}_k) < 0 \rightarrow A_k < 0$
  - $\mathbf{g}(\hat{\beta}_k) > 0 \rightarrow A_k > 0$


Iteration 3
Iteration 2
Iteration 1
(log-)Likelihood
Parameter Estimate

$$\mathbf{A}_\ell = \frac{\partial \ln L}{\partial \hat{\boldsymbol{\beta}}_\ell}$$

$$\hat{\boldsymbol{\beta}}_\ell = \hat{\boldsymbol{\beta}}_{\ell-1} + \frac{\partial \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}}$$


Two Likelihoods: Same Maximum,
Same First Derivative, Different
Second Derivatives

"Step Size"

$$\hat{\boldsymbol{\beta}}_{\ell} = \hat{\boldsymbol{\beta}}_{\ell-1} + \lambda_{\ell-1}\boldsymbol{\Delta}_{\ell-1}$$

- $\boldsymbol{\Delta} \rightarrow$ *direction*
- $\lambda \rightarrow$ *amount* ("step size")

Key: Hessian

$$\mathbf{H}(\hat{\boldsymbol{\beta}}) = \frac{\partial^2 \ln L}{\partial \hat{\boldsymbol{\beta}}^2}$$

How?

$$\begin{aligned} \hat{\boldsymbol{\beta}}_\ell &= \hat{\boldsymbol{\beta}}_{\ell-1} - \left(\frac{\partial^2 \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}^2} \right)^{-1} \frac{\partial \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}} \\ &= \hat{\boldsymbol{\beta}}_{\ell-1} - \mathbf{H}(\hat{\boldsymbol{\beta}}_{\ell-1})^{-1} \mathbf{g}(\hat{\boldsymbol{\beta}}_{\ell-1}) \end{aligned} \tag{1}$$

Sidebar: Newton-Raphson, re-revealed

Taylor series, anyone?

$$f(X) \approx f(a) + f'(a)(x - a)$$

Here,

$$\frac{\partial \ln L}{\partial \hat{\boldsymbol{\beta}}_\ell} \approx \frac{\partial \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}} + \frac{\partial^2 \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}^2}(\hat{\boldsymbol{\beta}}_\ell - \hat{\boldsymbol{\beta}}_{\ell-1})$$

What we really want...

$$\frac{\partial \ln L}{\partial \hat{\boldsymbol{\beta}}_\ell} = \mathbf{0}$$

So:

$$\mathbf{0} \approx \frac{\partial \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}} + \frac{\partial^2 \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}^2}(\hat{\boldsymbol{\beta}}_\ell - \hat{\boldsymbol{\beta}}_{\ell-1})$$

$$\begin{aligned}\hat{\boldsymbol{\beta}}_\ell &\approx \hat{\boldsymbol{\beta}}_{\ell-1} - \left(\frac{\partial^2 \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}^2}\right)^{-1} \frac{\partial \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}} \\ &\approx \hat{\boldsymbol{\beta}}_{\ell-1} - \mathbf{H}(\hat{\boldsymbol{\beta}}_{\ell-1})^{-1}\mathbf{g}(\hat{\boldsymbol{\beta}}_{\ell-1})\end{aligned}$$

Other Methods

Newton-Raphson requires $\mathbf{H}(\hat{\boldsymbol{\beta}})^{-1} \rightarrow$ *calculates* $\mathbf{H}(\hat{\boldsymbol{\beta}})^{-1}$ at every iteration. This can make it somewhat slow / computationally demanding.

Modified Marquardt:

- Used when $\mathbf{H}(\hat{\boldsymbol{\beta}})$ isn't invertable
- Adds a constant $\mathbf{C}$ to diag$[\mathbf{H}(\hat{\boldsymbol{\beta}})]$
- Variants: Add $\mathbf{C}(h_k)$

"Method of Scoring" (due to Fisher) uses:

$$\begin{aligned}
\hat{\boldsymbol{\beta}}_\ell &= \hat{\boldsymbol{\beta}}_{\ell-1} - \left[\mathsf{E}\left(\frac{\partial^2 \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}^2} \right)^{-1} \right] \frac{\partial \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}} \\
&= \hat{\boldsymbol{\beta}}_{\ell-1} - \{\mathsf{E}[\mathbf{H}(\hat{\boldsymbol{\beta}}_{\ell-1})]\}^{-1} \mathbf{g}(\hat{\boldsymbol{\beta}}_{\ell-1})
\end{aligned}$$

Berndt, Hall[2], and Hausman ("BHHH")

Uses:

$$\hat{\boldsymbol{\beta}}_{\ell} = \hat{\boldsymbol{\beta}}_{\ell-1} - \left(\sum_{i=1}^{N} \frac{\partial \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}} \frac{\partial \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}}' \right)^{-1} \frac{\partial \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}}$$

Advantages:

- (Relatively) very easy to compute
- Reasonably accurate...

Other "Newton Jr.s"

- Davidson-Fletcher-Powell ("DFP")
- Broyden et al. ("BFGS")
- They are:
  - Faster / more efficient
  - Comparatively bad at getting $-\left(\mathbf{H}(\hat{\boldsymbol{\beta}})\right)^{-1}$

Summary: Optimization & Inference

Method	"Step size" (∂^2) matrix	Variance-Covariance Estimate
Newton	Inverse of the observed second derivative (Hessian)	Inverse of the negative Hessian
Scoring	Inverse of the expected value of the Hessian (information matrix)	Inverse of the negative information matrix
BHHH	Outer product approximation of the information matrix	Inverse of the outer product approximation

Software Issues: R

Lots of optimizers:

- `maxLik` package: options for Newton-Raphson, BHHH, BFGS, others
- `optim` (in `stats`) – quasi-Newton, plus others
- `nlm` (in `stats`) – nonlinear minimization "using a Newton-type algorithm"
- `newton` (in `Bhat`) – Newton-Raphson solver
- `solveLP` (in `linprog`) – linear programming optimizer

R : Using `maxLik`

- *Must* provide log-likelihood function
- Can provide $\mathbf{H}(\hat{\boldsymbol{\beta}})$, $\mathbf{g}(\hat{\boldsymbol{\beta}})$, both, or neither
- Choose optimizer (Newton, BHHH, BFGS, etc.)
- Returns an object of class `maxLik`

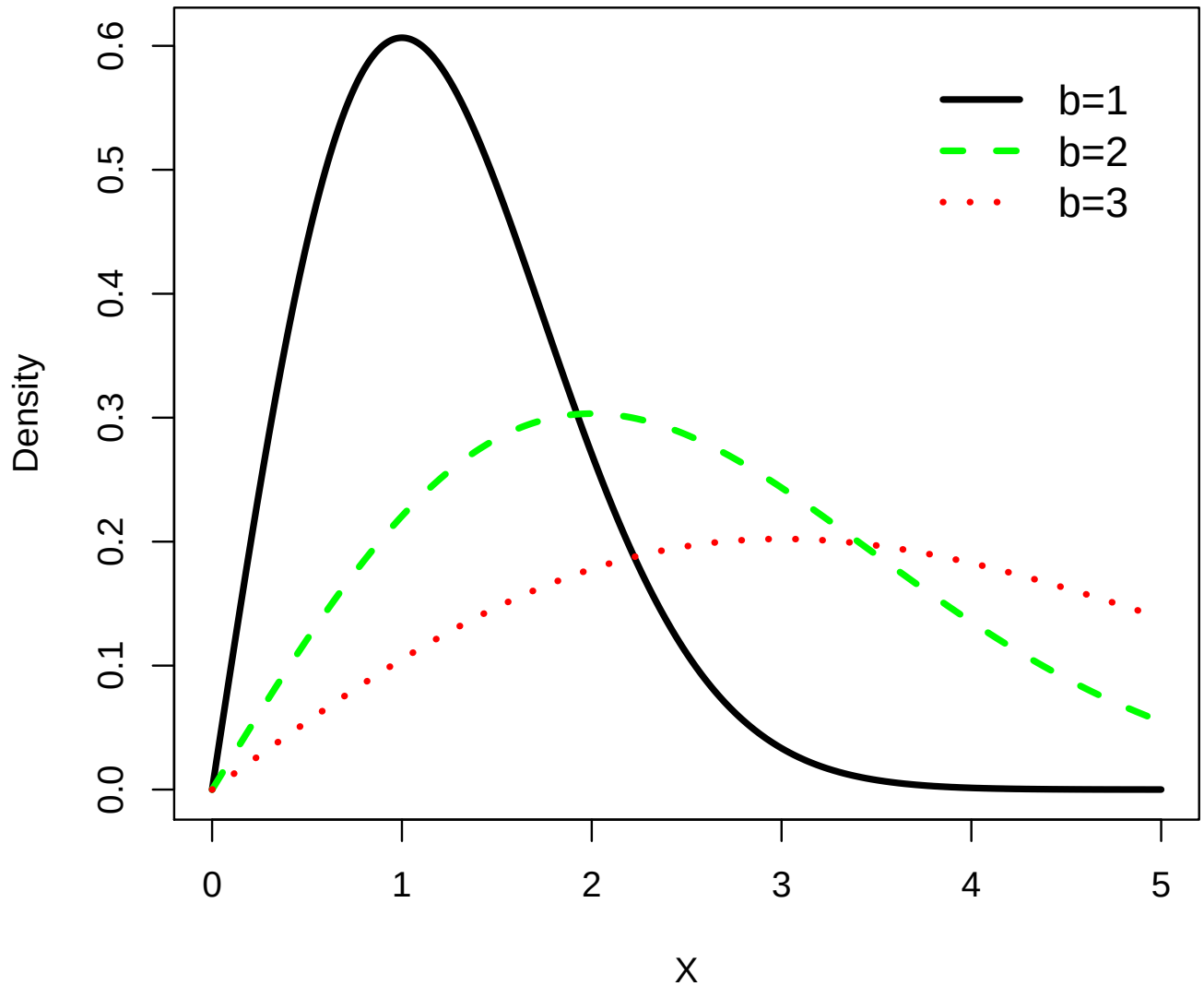
Rayleigh distribution density:

$$\Pr(X = x) = \frac{x}{b^2} \exp\left[\frac{-x^2}{2b^2}\right], \; b > 0$$

Other traits:

- Support $\in [0, \infty)$
- $E(X) = b\sqrt{\frac{\pi}{2}}$
- Mode $= b$
- $Var(X) = \frac{4-\pi}{2} b^2$

Rayleigh Densities



We can generate a Rayleigh-distributed random variable X with parameter b via inverse transform sampling, as:

$$X = b\sqrt{-2\ln(1-U)}$$

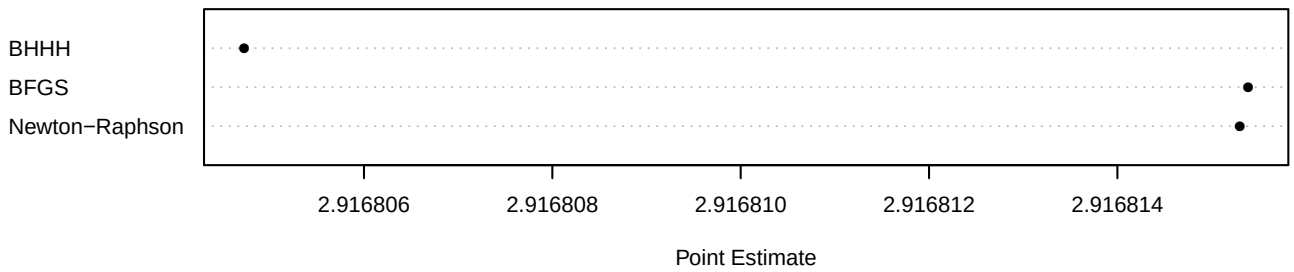
where $U \in \text{Uniform}[0,1]$. So, for (e.g.) $b = 3$:

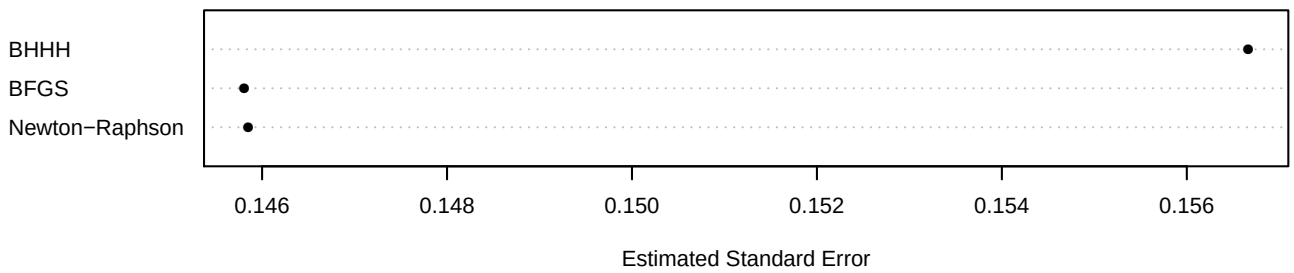
```
> library(maxLik,distr)
> set.seed(7222009)
> U<-runif(100)
> rayleigh<-3*sqrt(-2*log(1-U))  # b = 3
> loglike <- function(param) {
+    b <- param[1]
+    ll <- (log(x)-log(b^2)) + ((-x^2)/(2*b^2))
+    ll
+  }
```

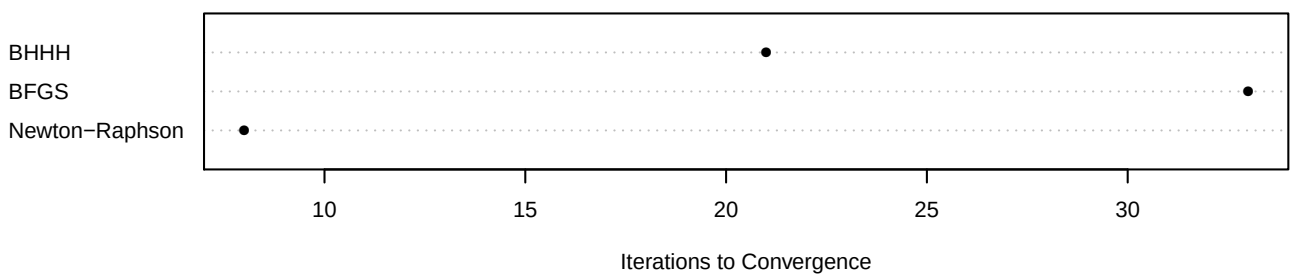
R : What We Like To See

```
> x<-rayleigh
> hats <- maxLik(loglike, start=c(1))
> summary(hats)
--------------------------------------------
Maximum Likelihood estimation
Newton-Raphson maximisation, 8 iterations
Return code 2: successive function values within tolerance limit
Log-Likelihood: -195.7921
1  free parameters
Estimates:
     Estimate Std. error t value Pr(> t)
[1,]   2.9168     0.1459      20  <2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1
--------------------------------------------
```

Comparing Optimizers







R : What We *Don't* Like To See

```
> Y<-c(0,0,0,0,0,1,1,1,1,1)
> X<-c(0,1,0,1,0,1,1,1,1,1)
> logL <- function(param) {
+   b0<-param[1]
+   b1<-param[2]
+   ll<-Y*log(exp(b0+b1*X)/(1+exp(b0+b1*X))) +
+       (1-Y)*log(1-(exp(b0+b1*X)/(1+exp(b0+b1*X))))
+   ll
+ }
```

R : What We *Don't* Like To See

```
> Bhat<-maxLik(logL,start=c(0,0))
> summary.maxLik(Bhat)
--------------------------------------------
Maximum Likelihood estimation
Newton-Raphson maximisation, 9 iterations
Return code 1: gradient close to zero
Log-Likelihood: -4.187887
2  free parameters
Estimates:
     Estimate Std. error t value Pr(> t)
[1,]   -104.3        Inf       0       1
[2,]    105.2        Inf       0       1
--------------------------------------------
```

Practical Optimization...

- Potential Problems
- Likely Causes
- Tips

Enemy # 1: Noninvertable $\mathbf{H}(\hat{\boldsymbol{\beta}})$

- "Non-concavity," "non-invertability," etc.
- (Some part of) the likelihood is "flat"
- Why? (Bob Dole...)

Problems

Identification

- Possible due to functional form alone...
- "Fragile"
- Manifestation: parameter instability

Poor Conditioning

- Numerical issues
- Potentially:
    - Collinearity
    - Other weirdnesses (nonlinearities)

Potential Causes

- Misspecification. SAD!
- Missing data
- Variable scaling
- Typical $\Pr(Y)$

Hints

- T-h-i-n-k!
- Know thy data
- Keep an eye on your iteration logs...
- Don't overreach