PLSC 503 – Spring 2021 Maximum Likelihood: Theory and Optimization

March 17, 2021

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

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

Some Data

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

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

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

So:

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

...

Recall that:

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

So:

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

More generally:

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

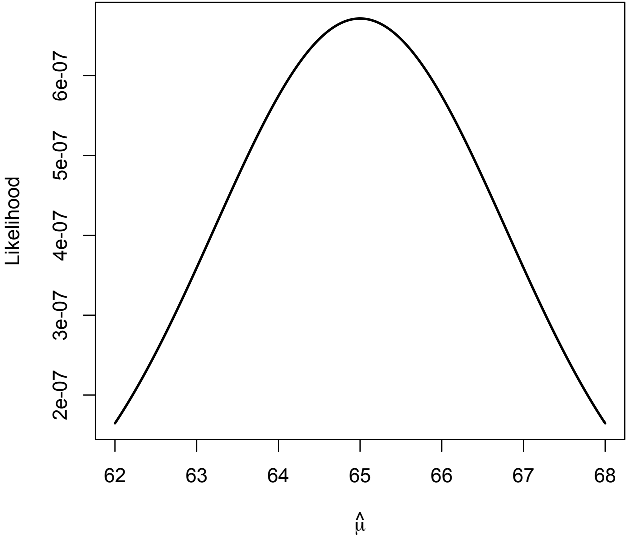
The *likelihood* is:

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

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

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

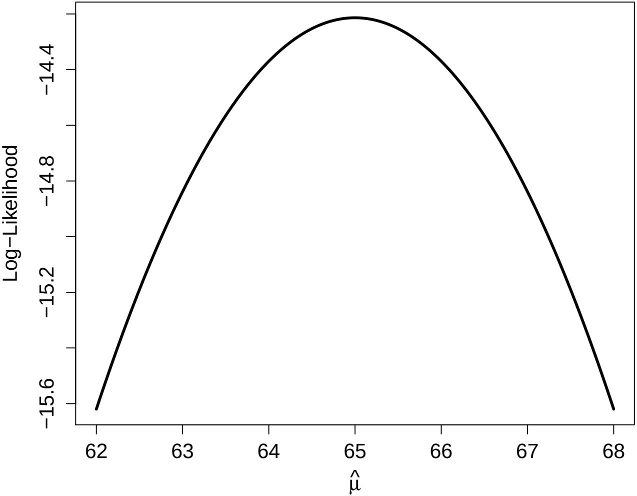
What a Likelihood Looks Like



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 $\frac{\partial^2 \ln L}{\partial \theta^2} < 0$.

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

Means:

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

Example: Normal Y (continued)

Solving yields:

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

Compare with:

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

Example: Linear Regression

Model:

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

Likelihood:

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

Log-likelihood:

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

"Kernel":

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

MLE in General

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

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

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

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

Digression: Taylor Series Approximation

For a $k+1$-times differentiable function $f(x)$, we can approximate the function at a with a *Taylor series approximation*:

$$\sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \cdots$$

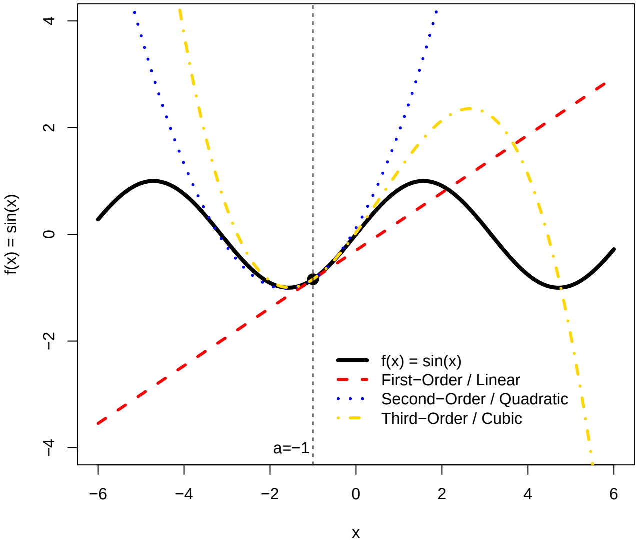
Special cases: First-order / linear:

$$f(x) \approx f(a) + \frac{f'(a)}{1!}(x-a)$$

Second-order / quadratic:

$$f(x) \approx f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2$$

Taylor Series, Illustrated



The gradient is:

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

First-order Taylor series approximation at θ:

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

Yields:

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

Need

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

So:

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

Yields:

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

Efficiency

Cramer-Rao say:

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

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

For MLE:

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

So,

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

By the Law of Large Numbers:

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

Or, equivalently:

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

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:

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

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

Optimization: Stuff We Won't Cover

- Grid search / "hill climbing"
- Genetic algorithms
- Annealing methods
- Local search methods (tabu, etc.)
- many others...

Find

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

Unconstrained optimization problem...

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...

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

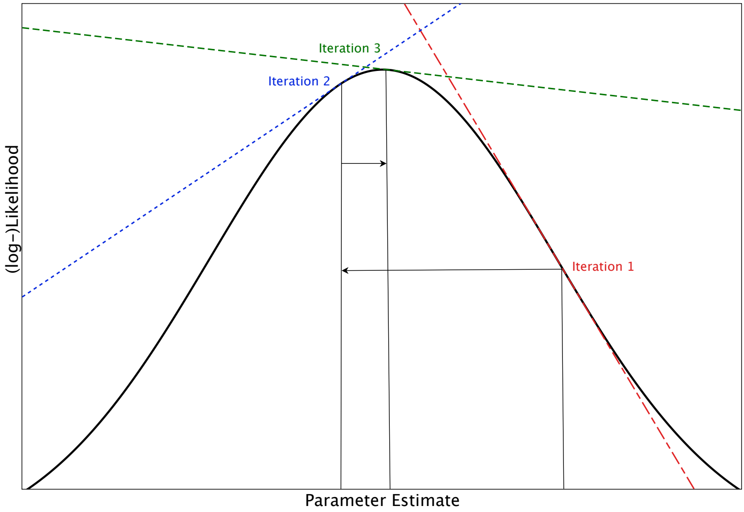
$$\hat{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}}_{\ell} \ni \hat{\boldsymbol{\beta}}_{\ell} - \hat{\boldsymbol{\beta}}_{\ell-1} (\equiv \mathsf{A}_{\ell}) < \tau$$

Key Question: What's $\mathbf{A}$?

One alternative:

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

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

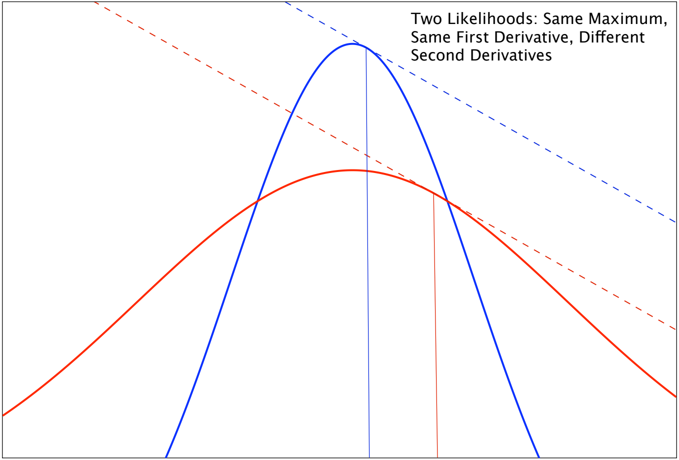

Iteration 3
Iteration 2
Iteration 1
(log−)Likelihood
Parameter Estimate

"Steepest Ascent"

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

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

A Challenge


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

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

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

Key: Hessian

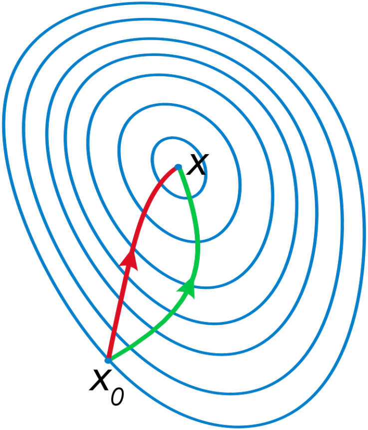
$$\mathbf{H}(\hat{\boldsymbol{\beta}}) = \frac{\partial^2 \ln L}{\partial \hat{\boldsymbol{\beta}}^2}$$

How?

$$\hat{\boldsymbol{\beta}}_\ell = \hat{\boldsymbol{\beta}}_{\ell-1} - \left(\frac{\partial^2 \ln L}{\partial \hat{\boldsymbol{\beta}}^2_{\ell-1}}\right)^{-1} \frac{\partial \ln L}{\partial \hat{\boldsymbol{\beta}}_{\ell-1}}$$

$$= \hat{\boldsymbol{\beta}}_{\ell-1} - [\mathbf{H}(\hat{\boldsymbol{\beta}}_{\ell-1})^{-1}\mathbf{g}(\hat{\boldsymbol{\beta}}_{\ell-1})]$$

Newton-Raphson vs. Steepest Ascent



(Source)

Sidebar: Newton-Raphson, re-revealed

Taylor series, anyone?

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

Here,

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

But we *really* want:

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

So:

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

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

Newton-Raphson

- Uses $\mathbf{H}(\hat{\boldsymbol{\beta}})^{-1}$ so
- *Calculates* $\mathbf{H}(\hat{\boldsymbol{\beta}})^{-1}$ at every iteration...

"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":

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

- Due to Fisher
- Advantages:
  - $\approx$ Newton-Raphson
  - <u>Can</u> be faster/simpler

Berndt, Hall^2, and Hausman ("BHHH"):

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

Advantages:

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

Other "Newton Jr.s":

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

Summary

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

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

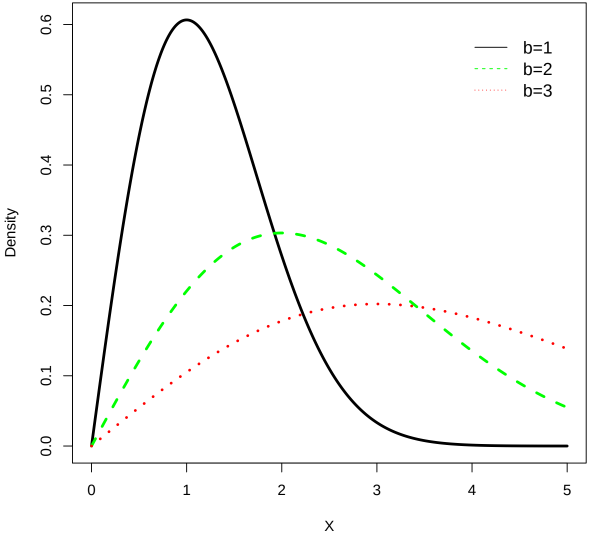
R : Using `maxLik`

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

Rayleigh distribution:

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

Some Rayleighs



R : What We Like To See

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

```
> 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
--------------------------------------------
```

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)

> xtabs(~X+Y)
   Y
X   0 1
  0 3 0
  1 2 5

> 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
--------------------------------------------
```

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

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

Other Potential Problems

Identification

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

Poor Conditioning

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

Potential Causes of Problems:

- Bad specification!
- 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