PLSC 503 – Spring 2022
Maximum Likelihood: Theory and Optimization

March 23, 2022

A Model:

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

$$\mathsf{E}(Y) = \mu$$
$$\mathsf{Var}(Y) = \sigma^2$$

Some data:

$$Y = \begin{array}{l} 64 \\ 63 \\ 59 \\ 71 \\ 68 \end{array}$$

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

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

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

...

Probabilities, Joint

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:

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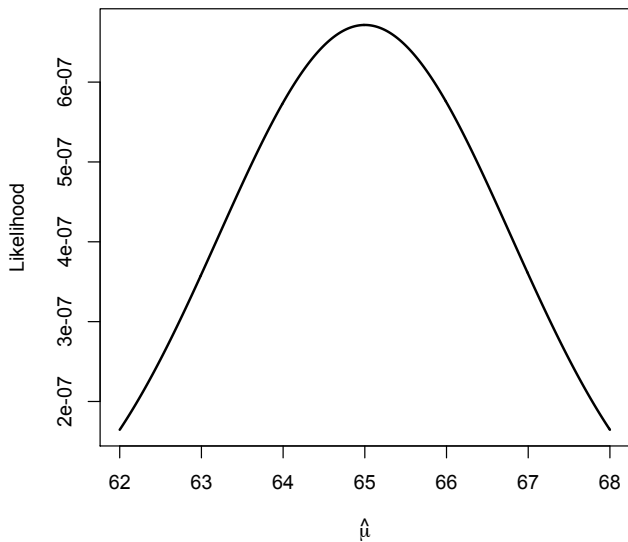\end{aligned}
$$

Likelihood

The *likelihood* is:

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

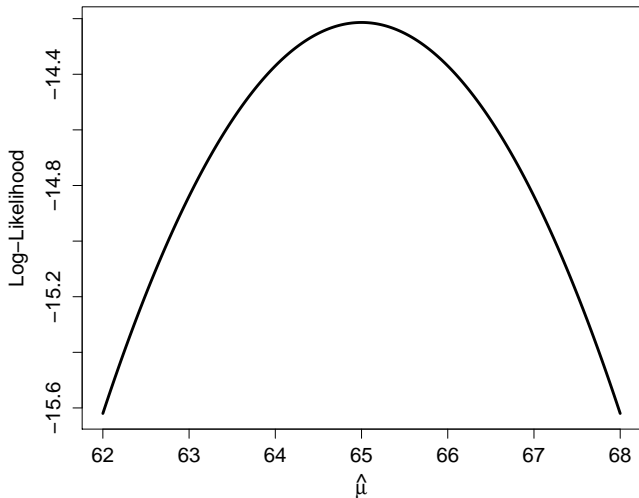For $\hat{\mu} = 68$ and $\hat{\sigma} = 4$, that means:

$$
\begin{aligned}
L &= \frac{1}{\sqrt{2\pi 16}} \exp\left[-\frac{(64-68)^2}{32} \right] \times \\
&\quad \frac{1}{\sqrt{2\pi 16}} \exp\left[-\frac{(63-68)^2}{32} \right] \times \\
&\quad \frac{1}{\sqrt{2\pi 16}} \exp\left[-\frac{(59-68)^2}{32} \right] \times \dots \\
&= 0.060 \times 0.046 \times 0.008 \times \dots \\
&= \text{some reeeeeally small number...}
\end{aligned}
$$

What a Likelihood Looks Like

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

What a Log-Likelihood Looks Like

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:

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

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

Compare with:

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

Example: Linear Regression

Model:

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

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":

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

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

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

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

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

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*:

$$\sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \cdots$$
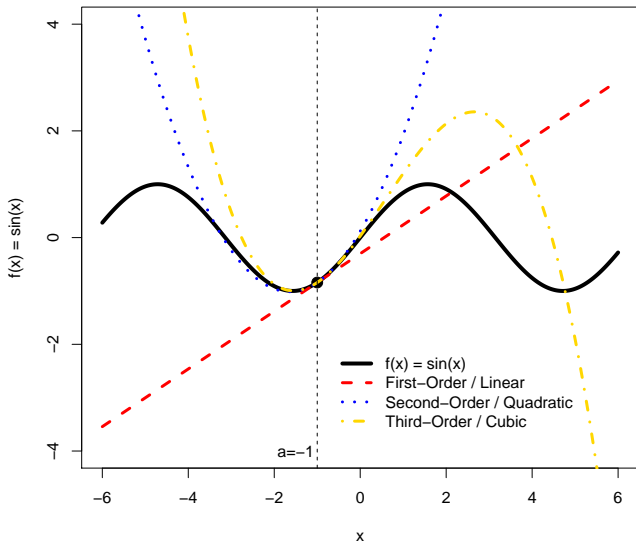
Special cases: First-order / linear:

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

Second-order / quadratic:

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

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

Yields:

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

Cramer-Rao *lower bound*:

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

For the MLE $\hat{\theta}$:

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

Under some easy regularity conditions:

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

So,

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

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

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

- Grid search / "hill climbing"

- Genetic algorithms

- Annealing methods

- Local search methods (tabu, etc.)

- many others...

Find

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

Unconstrained optimization problem...

Intuition:

- Start with $\hat{\boldsymbol{\beta}}_0$
- Adjust:

$$\hat{\boldsymbol{\beta}}_1 = \hat{\boldsymbol{\beta}}_0 + \mathbf{A}_0$$

- Repeat.

At each iteration:

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

Convergence:

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

One alternative:

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

Here, $\mathbf{g}(\hat{\boldsymbol{\beta}}) =$ "directionality" of change

- $\mathbf{g}(\hat{\beta}_k) < 0 \to A_k < 0$
- $\mathbf{g}(\hat{\beta}_k) > 0 \to A_k > 0$
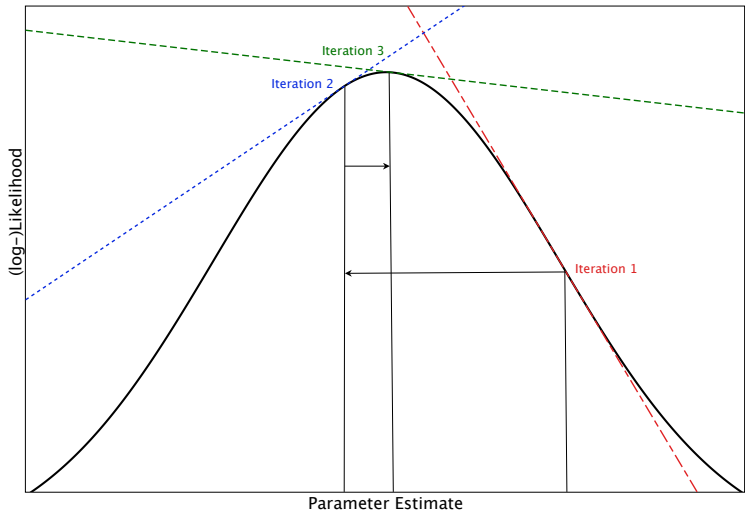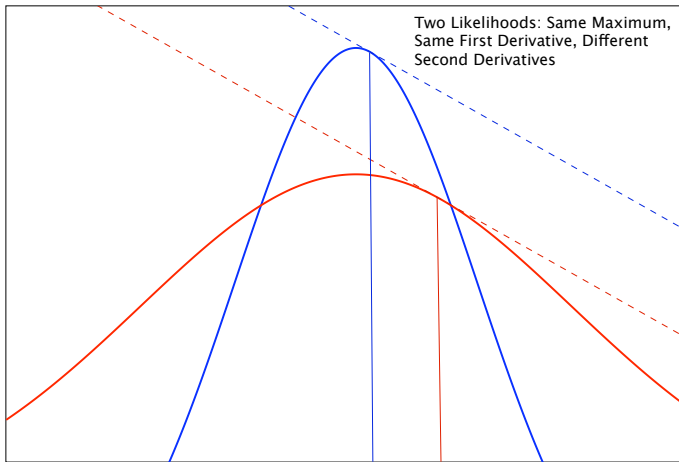
"Method of Steepest Ascent"

Adjust by the gradient:

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

At each iteration:

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

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

Generalize:

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

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

Key: Hessian

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

How?

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

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

(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:

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

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

- 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 $\text{diag}[\mathbf{H}(\hat{\boldsymbol{\beta}})]$
- Variants: Add $\mathbf{C}(h_k)$

Fisher's "Method of Scoring":

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

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 $-\left(\mathbf{H}(\hat{\boldsymbol{\beta}}) \right)^{-1}$

Method	"Step size" (∂^2) matrix	Variance-Covariance Estimate
Newton	Inverse of the observed second derivative (Hessian)	Inverse of the negative Hessian
Method of 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

- *Must* provide log-likelihood function
- Can provide $\mathbf{H}(\hat{\boldsymbol{\beta}})$, $\mathbf{g}(\hat{\boldsymbol{\beta}})$, both, or neither
- Can choose *starting values* for $\hat{\theta}$
- Choose optimizer (Newton, BHHH, BFGS, etc.)
- Can also set the maximum number of iterations, convergence tolerance τ, etc.
- Returns an object of class `maxLik`

Rayleigh distribution:

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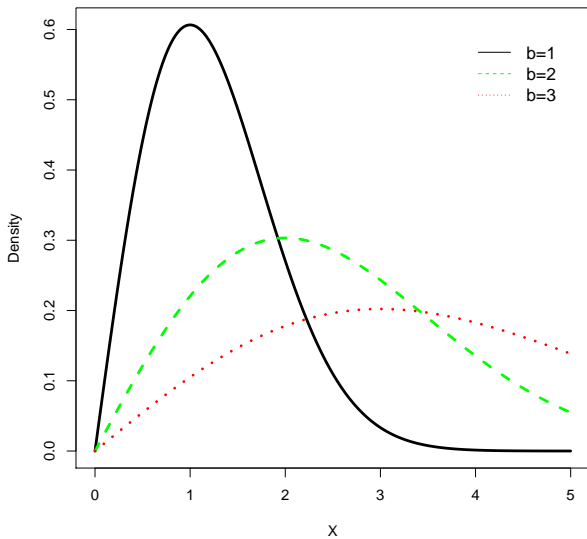
with $b > 0$.

For a Rayleigh-distributed variable X,

$$\bar{X} = b\sqrt{\frac{\pi}{2}} \approx 1.253 \times b$$

$$\text{Var}(X) = \left(\frac{4 - \pi}{2}\right) b^2 \approx 0.429 \times b^2$$

$$\text{mode}(X) = b$$

Because for the Rayleigh:

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

the log likelihood is:

$$
\begin{aligned}
lnL &= ln\prod_{i=1}^{N}\left\{\frac{X_i}{b^2}\exp\left[\frac{-X_i^2}{2b^2}\right]\right\} \\
&= \sum_{i=1}^{N}[ln(X_i) - ln(b^2)] + \left(\frac{-X_i^2}{2b^2}\right)
\end{aligned}
$$

R : What We Like To See

```
> library(maxLik,distr)
> set.seed(7222009)
> U<-runif(100)
> rayleigh<-3*sqrt(-2*log(1-U)) # Rayleigh with b = 3
> loglike <- function(param) {
+    b <- param[1]
+    ll <- (log(x)-log(b^2)) + ((-x^2)/(2*b^2)) # log-Lik
+    ll
+  }
```
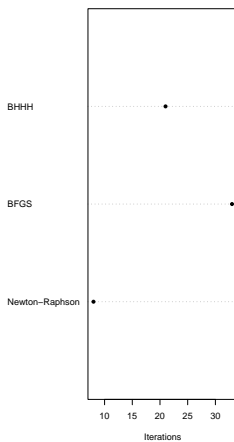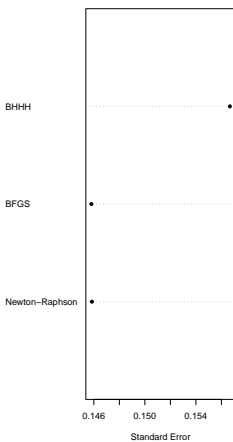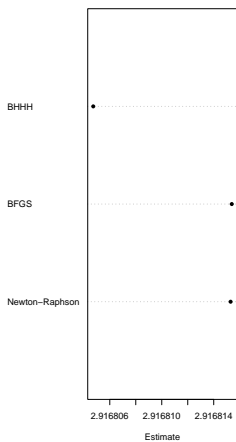
R : What We Like To See

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

The Rayleigh: Comparing Optimizers

```
> set.seed(7222009)
> bad<-runif(100)
> bad<-0.000001*sqrt(-2*log(1-bad))
> x<-bad
> hatsBad <- maxLik(loglike, start=c(1))
> summary(hatsBad)
--------------------------------------------
Maximum Likelihood estimation
Newton-Raphson maximisation, 8 iterations
Return code 3: Last step could not find a value above the current.
Boundary of parameter space?
Consider switching to a more robust optimisation method temporarily.
Log-Likelihood: 967.7
1  free parameters
Estimates:
      Estimate Std. error t value Pr(> t)
[1,] 0.0000082        NaN     NaN     NaN
--------------------------------------------
Warning messages:
1: In sqrt(diag(vc)) : NaNs produced
2: In sqrt(diag(vc)) : NaNs produced
```

R : What We *Don't* Like To See (Part II)

```
> set.seed(7222009)
> alsobad<-runif(100)
> alsobad<-999999999*sqrt(-2*log(1-alsobad))
> x<-alsobad
> hatsBad2 <- maxLik(loglike, start=c(1))
> summary(hatsBad2)
--------------------------------------------
Maximum Likelihood estimation
Newton-Raphson maximisation, 19 iterations
Return code 1: gradient close to zero (gradtol)
Log-Likelihood: -6706
1  free parameters
Estimates:
                Estimate         Std. error t value Pr(> t)
[1,] 12003488289174087680            Inf       0        1
--------------------------------------------
```

Potential Problems

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

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

Poor / "Fragile" Identification

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

Poor Conditioning

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

Practical Optimization

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