

PLSC 503 – Spring 2025

Maximum Likelihood: Theory and Optimization

March 24, 2025

A Toy Example

A Model:

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

$$E(Y) = \mu$$

$$\text{Var}(Y) = \sigma^2$$

Some data:

$$Y = 64$$

$$63$$

$$59$$

$$71$$

$$68$$

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

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

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

...

Recall that:

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

So:

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

More generally:

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

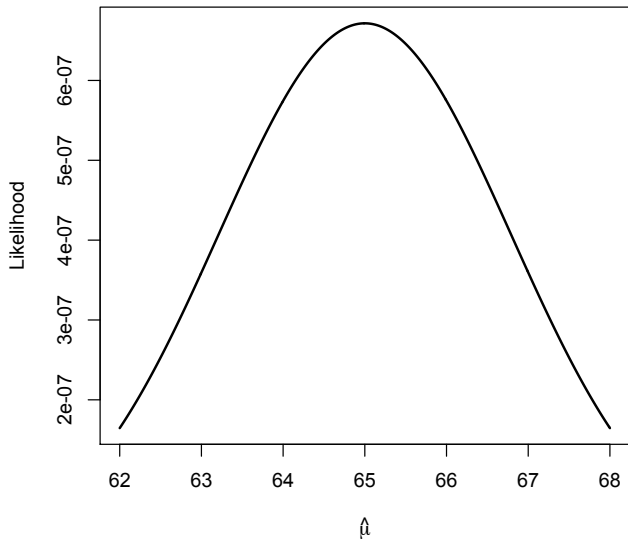
The *likelihood* is:

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

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

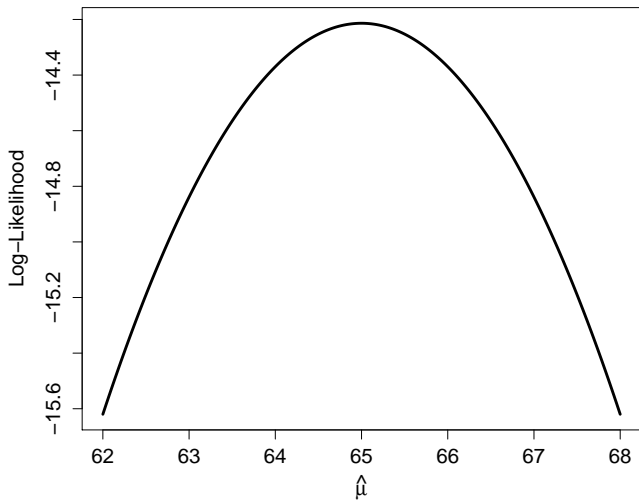
$$\begin{aligned} L &= \frac{1}{\sqrt{2\pi}16} \exp \left[-\frac{(64 - 68)^2}{32} \right] \times \\ &\quad \frac{1}{\sqrt{2\pi}16} \exp \left[-\frac{(63 - 68)^2}{32} \right] \times \\ &\quad \frac{1}{\sqrt{2\pi}16} \exp \left[-\frac{(59 - 68)^2}{32} \right] \times \dots \\ &= 0.060 \times 0.046 \times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

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



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

For a Normal distribution:

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

This means:

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

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

Example: Normal Y (continued)

Solving yields:

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

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

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”:

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

Probability density:

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

Likelihood:

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

Log-likelihood:

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

MLE is:

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

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*:

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

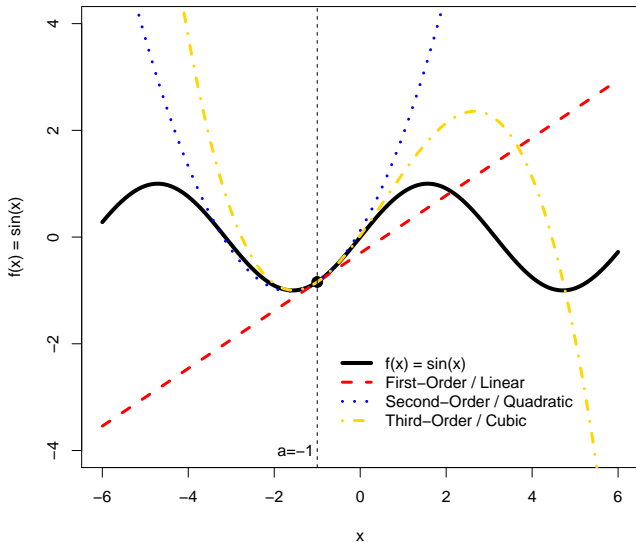
Special cases: First-order / linear:

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

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

Yields:

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

Cramer-Rao *lower bound*:

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

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

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

Under some easy regularity conditions:

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

So,

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

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: Things We Won't Cover

- Grid search / “hill climbing”
- Genetic algorithms
- Simulated annealing methods
- Local search methods (tabu, etc.)
- many others...

Find

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

Unconstrained optimization problem...

Intuition:

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

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

- Repeat.

At each iteration:

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

Convergence:

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

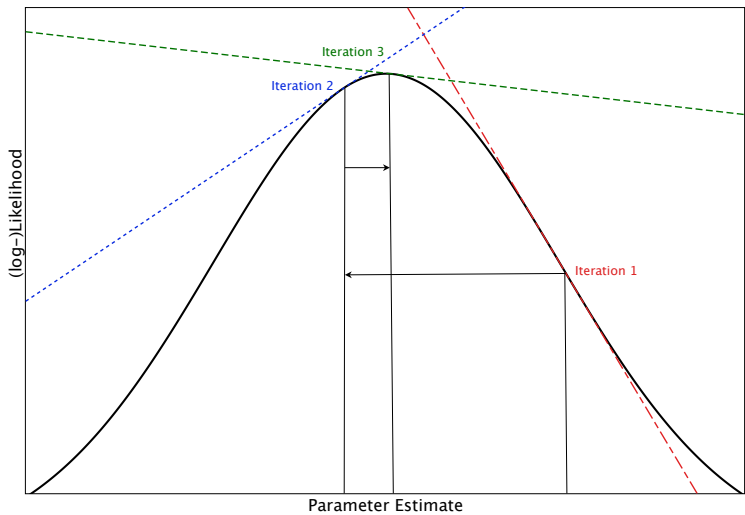
Key Question: What's **A**?

One alternative:

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

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

- $\mathbf{g}(\hat{\beta}_k) < 0 \rightarrow A_k < 0$
- $\mathbf{g}(\hat{\beta}_k) > 0 \rightarrow A_k > 0$



“Method of Steepest Ascent”

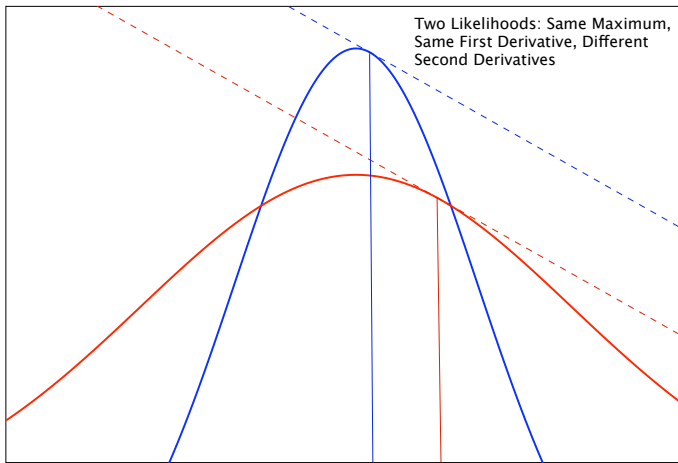
Adjust by the gradient:

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

At each iteration:

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

A Challenge



Generalize:

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

- $\Delta \rightarrow$ *direction*
- $\lambda \rightarrow$ *amount* (“step size”)

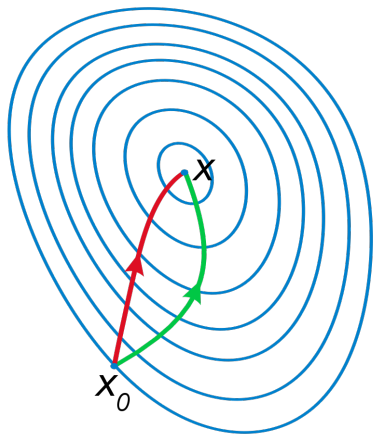
Key: Hessian

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

How?

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

Newton-Raphson vs. Steepest Ascent



(Source)

Sidebar: Newton-Raphson, re-revealed

Taylor series, anyone?

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

Here,

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

But we *really* want:

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

So:

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

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

The downside:

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



“Modified Marquardt”:

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

Fisher's “Method of Scoring”:

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

Advantages:

- \approx Newton-Raphson
- Can be faster/simpler

Berndt, Hall², and Hausman (“BHHH”):

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

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

Calculating $\widehat{\text{Var}}(\hat{\theta})$

Step Functions and Variances:

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

Details:

- *Must* provide log-likelihood function
- Can provide $\mathbf{H}(\hat{\beta})$, $\mathbf{g}(\hat{\beta})$, 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 ,

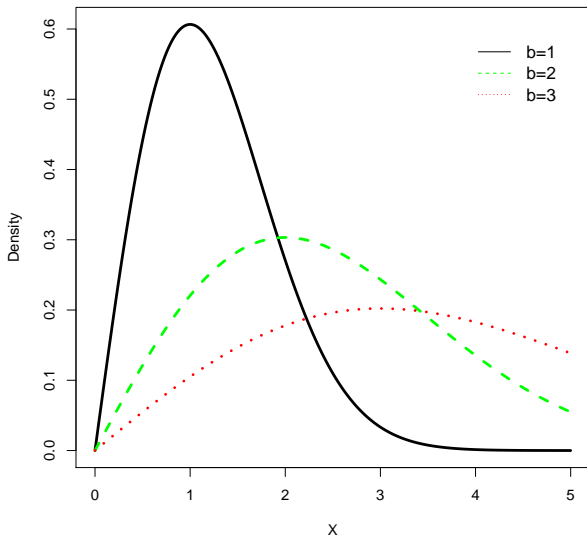
$$\bar{X} = b \sqrt{\frac{\pi}{2}} \approx 1.253 \times b$$

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

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



Some Rayleighs



Because for the Rayleigh:

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

the log likelihood is:

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

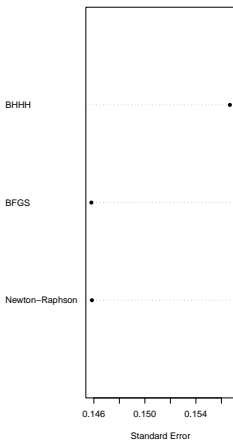
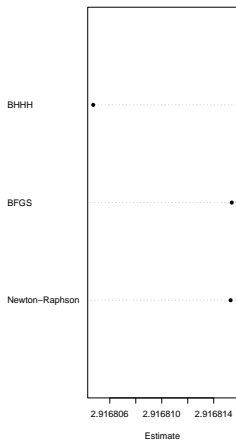
R : What We Like To See

```
> 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



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

```
> 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

```
-----
```

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

- “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)

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