# PLSC 503 – Spring 2018 Optimization

April 3, 2018

## Stuff We Won't Cover Today

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

### The Basic Problem

Find

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

Unconstrained optimization problem...

### The Intuition

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

$$\boldsymbol{\hat{eta}_1} = \boldsymbol{\hat{eta}_0} + \boldsymbol{\mathsf{A_0}}$$

Repeat.

## More Specifically...

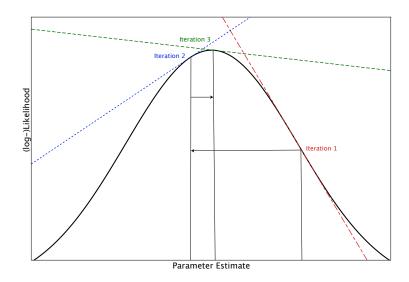
$$oldsymbol{\hat{eta}}_\ell = oldsymbol{\hat{eta}}_{\ell-1} + oldsymbol{\mathsf{A}}_{\ell-1}$$

$$\hat{oldsymbol{eta}} = \hat{oldsymbol{eta}}_\ell 
i \hat{oldsymbol{eta}}_\ell - \hat{oldsymbol{eta}}_{\ell-1} (\equiv oldsymbol{\mathsf{A}}_\ell) < au$$

### What's **A**?

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

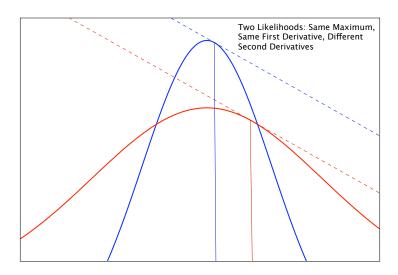
- $\mathbf{g}(\hat{oldsymbol{eta}}) =$  "directionality" of change
  - $\mathbf{g}(\hat{\beta}_k) < 0 \rightarrow A_k < 0$
  - $\mathbf{g}(\hat{\beta}_k) > 0 \rightarrow A_k > 0$



## "Steepest Ascent"

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

$$\hat{oldsymbol{eta}}_{\ell} = \hat{oldsymbol{eta}}_{\ell-1} + rac{\partial \ln L}{\partial \hat{oldsymbol{eta}}_{\ell-1}}$$



## "Step Size"

$$\hat{oldsymbol{eta}}_{\ell} = \hat{oldsymbol{eta}}_{\ell-1} + \lambda_{\ell-1} oldsymbol{\Delta}_{\ell-1}$$

- $\Delta \rightarrow direction$
- $\lambda \rightarrow$  amount ("step size")

## Key: Hessian

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

How?

## Newton-Raphson

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

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

## Sidebar: Newton-Raphson, re-revealed

Taylor series, anyone?

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

Here,

$$rac{\partial \ln L}{\partial \hat{oldsymbol{eta}}_{\ell}} \; pprox \; rac{\partial \ln L}{\partial \hat{oldsymbol{eta}}_{\ell-1}} + rac{\partial^2 \ln L}{\partial \hat{oldsymbol{eta}}_{\ell-1}^2} (\hat{oldsymbol{eta}}_{\ell} - \hat{oldsymbol{eta}}_{\ell-1})$$

## What we really want...

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

### Punch Line

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

$$egin{aligned} \hat{oldsymbol{eta}}_{\ell} &pprox & \hat{oldsymbol{eta}}_{\ell-1} - \left(rac{\partial^2 \ln L}{\partial \hat{oldsymbol{eta}}_{\ell-1}^2}
ight)^{-1} rac{\partial \ln L}{\partial \hat{oldsymbol{eta}}_{\ell-1}} \ &pprox & \hat{oldsymbol{eta}}_{\ell-1} - \mathbf{H}(\hat{oldsymbol{eta}}_{\ell-1})^{-1} \mathbf{g}(\hat{oldsymbol{eta}}_{\ell-1}) \end{aligned}$$

## Newton-Raphson

- Uses  $\mathbf{H}(\hat{eta})^{-1}$  so
- Calculates  $\mathbf{H}(\hat{\boldsymbol{\beta}})^{-1}$ .



## Modified Marquardt

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

## "Method of Scoring"

Uses:

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

$$= \hat{\boldsymbol{\beta}}_{\ell-1} - \{ \mathsf{E} [\mathbf{H} (\hat{\boldsymbol{\beta}}_{\ell-1})] \}^{-1} \mathbf{g} (\hat{\boldsymbol{\beta}}_{\ell-1})$$
(2)

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

## Berndt, Hall<sup>2</sup>, 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:
  - Very fast/efficient
  - Pretty bad at getting  $-\left(\mathbf{H}(\hat{eta})\right)^{-1}$

## Summary

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

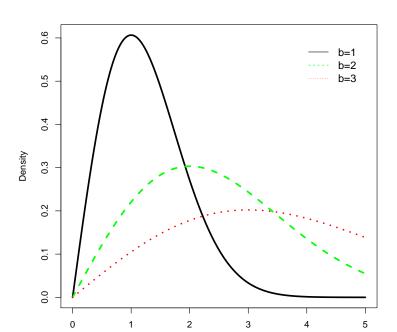
### R: Using maxLik

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

## R : Examples

Rayleigh distribution:

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



### 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]
+    l1 <- (log(x)-log(b^2)) + ((-x^2)/(2*b^2))
+    l1
+ }</pre>
```

### R: What We Like To See

```
> x<-rayleigh
> hats <- maxLik(loglike, start=c(1))</pre>
> 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)
> logL <- function(param) {
+ b0<-param[1]
+ b1<-param[2]
+ l1<-Y*log(exp(b0+b1*X)/(1+exp(b0+b1*X))) +
+ (1-Y)*log(1-(exp(b0+b1*X)/(1+exp(b0+b1*X))))
+ l1
+ }</pre>
```

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

```
> Bhat<-maxLik(logL,start=c(0,0))</pre>
> 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
[2,] 105.2 Inf
```

## Practical Optimization...

- Potential Problems
- Likely Causes
- Tips

### **Problems**

### 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

- 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