## Large Sample Theory

Study approximate behaviour of  $\widehat{\theta}$  by studying the function U.

Notice U is sum of independent random variables.

**Theorem**: If  $Y_1, Y_2, \ldots$  are iid with mean  $\mu$  then

$$\frac{\sum Y_i}{n} \to \mu$$

Called law of large numbers. Strong law

$$P(\lim \frac{\sum Y_i}{n} = \mu) = 1$$

and the weak law that

$$\lim P(|\frac{\sum Y_i}{n} - \mu| > \epsilon) = 0$$

For iid  $Y_i$  the stronger conclusion holds; for our heuristics ignore differences between these notions.

Now suppose  $\theta_0$  is true value of  $\theta$ . Then

$$U(\theta)/n \to \mu(\theta)$$

where

$$\mu(\theta) = E_{\theta_0} \left[ \frac{\partial \log f}{\partial \theta} (X_i, \theta) \right]$$
$$= \int \frac{\partial \log f}{\partial \theta} (x, \theta) f(x, \theta_0) dx$$

**Example**:  $N(\mu, 1)$  data:

$$U(\mu)/n = \sum (X_i - \mu)/n = \bar{X} - \mu$$

If the true mean is  $\mu_0$  then  $\bar{X} \to \mu_0$  and

$$U(\mu)/n \to \mu_0 - \mu$$

Consider  $\mu < \mu_0$ : derivative of  $\ell(\mu)$  is likely to be positive so that  $\ell$  increases as  $\mu$  increases.

For  $\mu > \mu_0$ : derivative is probably negative and so  $\ell$  tends to be decreasing for  $\mu > 0$ .

Hence:  $\ell$  is likely to be maximized close to  $\mu_0$ .

Repeat ideas for more general case. Study rv

$$\log[f(X_i,\theta)/f(X_i,\theta_0)].$$

You know the inequality

$$E(X)^2 \leq E(X^2)$$

(difference is  $Var(X) \ge 0$ .)

Generalization: Jensen's inequality: for g a convex function  $(g'' \ge 0 \text{ roughly})$  then

$$g(E(X)) \le E(g(X))$$

Inequality above has  $g(x) = x^2$ . Use  $g(x) = -\log(x)$ : convex because  $g''(x) = x^{-2} > 0$ . We get

$$-\log(E_{\theta_0}[f(X_i,\theta)/f(X_i,\theta_0)]$$

$$\leq E_{\theta_0}[-\log\{f(X_i,\theta)/f(X_i,\theta_0)\}]$$

But

$$E_{\theta_0} \left[ \frac{f(X_i, \theta)}{f(X_i, \theta_0)} \right] = \int \frac{f(x, \theta)}{f(x, \theta_0)} f(x, \theta_0) dx$$
$$= \int f(x, \theta) dx$$
$$= 1$$

We can reassemble the inequality and this calculation to get

$$E_{\theta_0}[\log\{f(X_i,\theta)/f(X_i,\theta_0)\}] \le 0$$

Fact: inequality is strict unless the  $\theta$  and  $\theta_0$  densities are actually the same.

Let  $\mu(\theta) < 0$  be this expected value.

Then for each  $\theta$  we find

$$\frac{\ell(\theta) - \ell(\theta_0)}{n} = \frac{\sum \log[f(X_i, \theta) / f(X_i, \theta_0)]}{n} \rightarrow \mu(\theta)$$

This proves likelihood probably higher at  $\theta_0$  than at any other single  $\theta$ .

Idea can often be stretched to prove that the mle is **consistent**; need **uniform** convergence in  $\theta$ .

**Definition** A sequence  $\hat{\theta}_n$  of estimators of  $\theta$  is consistent if  $\hat{\theta}_n$  converges weakly (or strongly) to  $\theta$ .

**Proto theorem**: In regular problems the mle  $\hat{\theta}$  is consistent.

More precise statements of possible conclusions. Use notation

$$N(\epsilon) = \{\theta : |\theta - \theta_0| \le \epsilon\}.$$

Suppose:

 $\widehat{\theta}_n$  is global maximizer of  $\ell$ .

 $\widehat{\theta}_{n,\delta}$  maximizes  $\ell$  over  $N(\delta) = \{ |\theta - \theta_0| \leq \delta \}$ .

$$A_{\epsilon} = \{|\widehat{\theta}_n - \theta_0| \le \epsilon\}$$

$$B_{\delta,\epsilon} = \{|\widehat{\theta}_{n,\delta} - \theta_0| \le \epsilon\}$$

$$C_L = \{\exists ! \theta \in N(L/n^{1/2}) : U(\theta) = 0, U'(\theta) < 0\}$$

#### Theorem:

- 1. Under conditions **I**  $P(A_{\epsilon}) \rightarrow 1$  for each  $\epsilon > 0$ .
- 2. Under conditions **II** there is a  $\delta > 0$  such that for all  $\epsilon > 0$  we have  $P(B_{\delta,\epsilon}) \to 1$ .
- 3. Under conditions **III** for all  $\delta > 0$  there is an L so large and an  $n_0$  so large that for all  $n \geq n_0$ ,  $P(C_L) > 1 \delta$ .
- 4. Under conditions **III** there is a sequence  $L_n$  tending to  $\infty$  so slowly that  $P(C_{L_n}) \to 1$ .

Point: conditions get weaker as conclusions get weaker. Many possible conditions in literature. See book by Zacks for some precise conditions.

## **Asymptotic Normality**

Study shape of log likelihood near the true value of  $\theta$ .

Assume  $\hat{\theta}$  is a root of the likelihood equations close to  $\theta_0$ .

Taylor expansion (1 dimensional parameter  $\theta$ ):

$$U(\widehat{\theta}) = 0$$

$$= U(\theta_0) + U'(\theta_0)(\widehat{\theta} - \theta_0) + U''(\widetilde{\theta})(\widehat{\theta} - \theta_0)^2/2$$

for some  $\tilde{\theta}$  between  $\theta_0$  and  $\hat{\theta}$ .

WARNING: This form of the remainder in Taylor's theorem is not valid for multivariate  $\theta$ .

Derivatives of U are sums of n terms.

So each derivative should be proportional to n in size.

Second derivative is multiplied by the square of the small number  $\hat{\theta} - \theta_0$  so should be negligible compared to the first derivative term.

Ignoring second derivative term get

$$-U'(\theta_0)(\widehat{\theta}-\theta_0)\approx U(\theta_0)$$

Now look at terms U and U'.

Normal case:

$$U(\theta_0) = \sum (X_i - \mu_0)$$

has a normal distribution with mean 0 and variance n (SD  $\sqrt{n}$ ).

Derivative is

$$U'(\mu) = -n.$$

Next derivative U'' is 0.

Notice: both U and U' are sums of iid random variables.

Let

$$U_i = \frac{\partial \log f}{\partial \theta}(X_i, \theta_0)$$

and

$$V_i = -\frac{\partial^2 \log f}{\partial \theta^2}(X_i, \theta)$$

In general,  $U(\theta_0) = \sum U_i$  has mean 0 and approximately a normal distribution.

Here is how we check that:

$$E_{\theta_0}(U(\theta_0)) = nE_{\theta_0}(U_1)$$

$$= n \int \frac{\partial \log(f(x, \theta_0))}{\partial \theta} f(x, \theta_0) dx$$

$$= n \int \frac{\partial f(x, \theta_0)/\partial \theta}{f(x, \theta_0)} f(x, \theta_0) dx$$

$$= n \int \frac{\partial f}{\partial \theta} (x, \theta_0) dx$$

$$= n \frac{\partial}{\partial \theta} \int f(x, \theta) dx \Big|_{\theta = \theta_0}$$

$$= n \frac{\partial}{\partial \theta} 1$$

$$= 0$$

Notice: interchanged order of differentiation and integration at one point.

This step is usually justified by applying the dominated convergence theorem to the definition of the derivative.

Differentiate identity just proved:

$$\int \frac{\partial \log f}{\partial \theta}(x,\theta) f(x,\theta) dx = 0$$

Take derivative of both sides wrt  $\theta$ ; pull derivative under integral sign:

$$\int \frac{\partial}{\partial \theta} \left[ \frac{\partial \log f}{\partial \theta} (x, \theta) f(x, \theta) \right] dx = 0$$

Do the derivative and get

$$-\int \frac{\partial^2 \log(f)}{\partial \theta^2} f(x,\theta) dx$$

$$= \int \frac{\partial \log f}{\partial \theta} (x,\theta) \frac{\partial f}{\partial \theta} (x,\theta) dx$$

$$= \int \left[ \frac{\partial \log f}{\partial \theta} (x,\theta) \right]^2 f(x,\theta) dx$$

### **Definition**: The **Fisher Information** is

$$I(\theta) = -E_{\theta}(U'(\theta)) = nE_{\theta_0}(V_1)$$

We refer to  $\mathcal{I}(\theta_0) = E_{\theta_0}(V_1)$  as the information in 1 observation.

The idea is that I is a measure of how curved the log likelihood tends to be at the true value of  $\theta$ . Big curvature means precise estimates. Our identity above is

$$I(\theta) = Var_{\theta}(U(\theta)) = n\mathcal{I}(\theta)$$

Now we return to our Taylor expansion approximation

$$-U'(\theta_0)(\widehat{\theta}-\theta_0)\approx U(\theta_0)$$

and study the two appearances of U.

We have shown that  $U = \sum U_i$  is a sum of iid mean 0 random variables. The central limit theorem thus proves that

$$n^{-1/2}U(\theta_0) \Rightarrow N(0, \sigma^2)$$

where  $\sigma^2 = Var(U_i) = E(V_i) = \mathcal{I}(\theta)$ .

Next observe that

$$-U'(\theta) = \sum V_i$$

where again

$$V_i = -\frac{\partial U_i}{\partial \theta}$$

The law of large numbers can be applied to show

$$-U'(\theta_0)/n \to E_{\theta_0}[V_1] = \mathcal{I}(\theta_0)$$

Now manipulate our Taylor expansion as follows

$$n^{1/2}(\widehat{\theta} - \theta_0) \approx \left[\frac{\sum V_i}{n}\right]^{-1} \frac{\sum U_i}{\sqrt{n}}$$

Apply Slutsky's Theorem to conclude that the right hand side of this converges in distribution to  $N(0, \sigma^2/\mathcal{I}(\theta)^2)$  which simplifies, because of the identities, to  $N\{0, 1/\mathcal{I}(\theta)\}$ .

## **Summary**

In regular families: assuming  $\hat{\theta} = \hat{\theta}_n$  is a consistent root of  $U(\theta) = 0$ .

•  $n^{-1/2}U(\theta_0) \Rightarrow MVN(0,\mathcal{I})$  where

$$\mathcal{I}_{ij} = \mathsf{E}_{\theta_0} \left\{ V_{1,ij}(\theta_0) \right\}$$

and

$$V_{k,ij}(\theta) = -\frac{\partial^2 \log f(X_k, \theta)}{\partial \theta_i \partial \theta_j}$$

ullet If  $\mathbf{V}_k( heta)$  is the matrix  $[V_{k,ij}]$  then

$$\frac{\sum_{k=1}^{n} \mathbf{V}_k(\theta_0)}{n} \to \mathcal{I}$$

• If  $V(\theta) = \sum_k V_k(\theta)$  then

$$\{\mathbf{V}(\theta_0)/n\}n^{1/2}(\widehat{\theta}-\theta_0)-n^{-1/2}U(\theta_0)\to 0$$

in probability as  $n \to \infty$ .

Also

$$\{V(\widehat{\theta})/n\}n^{1/2}(\widehat{\theta}-\theta_0)-n^{-1/2}U(\theta_0)\to 0$$
 in probability as  $n\to\infty$ .

- $n^{1/2}(\widehat{\theta} \theta_0) \{\mathcal{I}(\theta_0)\}^{-1}U(\theta_0) \to 0$  in probability as  $n \to \infty$ .
- $n^{1/2}(\widehat{\theta} \theta_0) \Rightarrow MVN(0, \mathcal{I}^{-1}).$
- In general (not just iid cases)

$$\sqrt{I(\theta_0)}(\widehat{\theta} - \theta_0) \Rightarrow N(0, 1)$$

$$\sqrt{I(\widehat{\theta})}(\widehat{\theta} - \theta_0) \Rightarrow N(0, 1)$$

$$\sqrt{V(\theta_0)}(\widehat{\theta} - \theta_0) \Rightarrow N(0, 1)$$

$$\sqrt{V(\widehat{\theta})}(\widehat{\theta} - \theta_0) \Rightarrow N(0, 1)$$

where  $V = -\ell''$  is the so-called *observed* information, the negative second derivative of the log-likelihood.

**Note**: If the square roots are replaced by matrix square roots we can let  $\theta$  be vector valued and get MVN(0,I) as the limit law.

Why all these different forms? Use limit laws to test hypotheses and compute confidence intervals. Test  $H_o$ :  $\theta = \theta_0$  using one of the 4 quantities as test statistic. Find confidence intervals using quantities as *pivots*. E.g.: second and fourth limits lead to confidence intervals

$$\widehat{\theta} \pm z_{\alpha/2} / \sqrt{I(\widehat{\theta})}$$

and

$$\hat{\theta} \pm z_{\alpha/2} / \sqrt{V(\hat{\theta})}$$

respectively. The other two are more complicated. For iid  $N(0,\sigma^2)$  data we have

$$V(\sigma) = \frac{3\sum X_i^2}{\sigma^4} - \frac{n}{\sigma^2}$$

and

$$I(\sigma) = \frac{2n}{\sigma^2}$$

The first line above then justifies confidence intervals for  $\sigma$  computed by finding all those  $\sigma$  for which

$$\left| \frac{\sqrt{2n}(\hat{\sigma} - \sigma)}{\sigma} \right| \le z_{\alpha/2}$$

Similar interval can be derived from 3rd expression, though this is much more complicated.

Usual summary: mle is consistent and asymptotically normal with an asymptotic variance which is the inverse of the Fisher information.

#### Problems with maximum likelihood

- 1. Many parameters lead to poor approximations. MLEs can be far from right answer. See homework for Neyman Scott example where MLE is not consistent.
- 2. Multiple roots of the likelihood equations: you must choose the right root. Start with different, consistent, estimator; apply iterative scheme like Newton Raphson to likelihood equations to find MLE. Not many steps of NR generally required if starting point is a reasonable estimate.

# Finding (good) preliminary Point Estimates

#### **Method of Moments**

Basic strategy: set sample moments equal to population moments and solve for the parameters.

**Definition**: The  $r^{\text{th}}$  sample moment (about the origin) is

$$\frac{1}{n} \sum_{i=1}^{n} X_i^r$$

The  $r^{\text{th}}$  population moment is

$$\mathsf{E}(X^r)$$

(Central moments are

$$\frac{1}{n} \sum_{i=1}^{n} (X_i - \bar{X})^r$$

and

$$E[(X-\mu)^r]$$
.

If we have p parameters we can estimate the parameters  $\theta_1, \dots, \theta_p$  by solving the system of p equations:

$$\mu_1 = \bar{X}$$

$$\mu_1 = \bar{X}$$

$$\mu_2' = \overline{X^2}$$

and so on to

$$\mu_p' = \overline{X^p}$$

You need to remember that the population moments  $\mu_k'$  will be formulas involving the parameters.

## Gamma Example

The Gamma $(\alpha, \beta)$  density is

$$f(x; \alpha, \beta) = \frac{1}{\beta \Gamma(\alpha)} \left(\frac{x}{\beta}\right)^{\alpha - 1} \exp\left[-\frac{x}{\beta}\right] \mathbf{1}(x > 0)$$

and has

$$\mu_1 = \alpha \beta$$

and

$$\mu_2' = \alpha(\alpha + 1)\beta^2.$$

This gives the equations

$$\alpha\beta = \overline{X}$$
$$\alpha(\alpha + 1)\beta^2 = \overline{X^2}$$

or

$$\alpha \beta = \overline{X}$$
$$\alpha \beta^2 = \overline{X^2} - \overline{X}^2.$$

Divide the second equation by the first to find the method of moments estimate of  $\beta$  is

$$\tilde{\beta} = (\overline{X^2} - \overline{X}^2)/\overline{X}.$$

Then from the first equation get

$$\tilde{\alpha} = \overline{X}/\tilde{\beta} = (\overline{X})^2/(\overline{X^2} - \overline{X}^2)$$
.

The method of moments equations are much easier to solve than the likelihood equations which involve the function

$$\psi(\alpha) = \frac{d}{d\alpha} \log(\Gamma(\alpha))$$

called the digamma function.

Score function has components

$$U_{\beta} = \frac{\sum X_i}{\beta^2} - n\alpha/\beta$$

and

$$U_{\alpha} = -n\psi(\alpha) + \sum \log(X_i) - n \log(\beta).$$

You can solve for  $\beta$  in terms of  $\alpha$  to leave you trying to find a root of the equation

$$-n\psi(\alpha) + \sum \log(X_i) - n \log(\sum X_i/(n\alpha)) = 0$$

To use Newton Raphson on this you begin with the preliminary estimate  $\hat{\alpha}_1 = \tilde{\alpha}$  and then compute iteratively

$$\hat{\alpha}_{k+1} = \frac{\overline{\log(X)} - \psi(\hat{\alpha}_k) - \log(\overline{X})/\hat{\alpha}_k}{1/\alpha - \psi'(\hat{\alpha}_k)}$$

until the sequence converges. Computation of  $\psi'$ , the trigamma function, requires special software. Web sites like *netlib* and *statlib* are good sources for this sort of thing.

## **Estimating Equations**

Same large sample ideas arise whenever estimates derived by solving some equation.

Example: large sample theory for **Generalized Linear Models**.

Suppose  $Y_i$  is number of cancer cases in some group of people characterized by values  $x_i$  of some covariates.

Think of  $x_i$  as containing variables like age, or a dummy for sex or average income or . . . .

Possible parametric regression model:  $Y_i$  has a Poisson distribution with mean  $\mu_i$  where the mean  $\mu_i$  depends somehow on  $x_i$ .

Typically assume  $g(\mu_i) = \beta_0 + x_i\beta$ ; g is **link** function.

Often  $g(\mu) = \log(\mu)$  and  $x_i\beta$  is a matrix product:  $x_i$  row vector,  $\beta$  column vector.

"Linear regression model with Poisson errors".

Special case  $log(\mu_i) = \beta x_i$  where  $x_i$  is a scalar.

The log likelihood is simply

$$\ell(\beta) = \sum (Y_i \log(\mu_i) - \mu_i)$$

ignoring irrelevant factorials. The score function is, since  $log(\mu_i) = \beta x_i$ ,

$$U(\beta) = \sum (Y_i x_i - x_i \mu_i) = \sum x_i (Y_i - \mu_i)$$

(Notice again that the score has mean 0 when you plug in the true parameter value.)

The key observation, however, is that it is not necessary to believe that  $Y_i$  has a Poisson distribution to make solving the equation U=0 sensible. Suppose only that  $\log(E(Y_i))=x_i\beta$ . Then we have assumed that

$$E_{\beta}(U(\beta)) = 0$$

This was the key condition in proving that there was a root of the likelihood equations which was consistent and here it is what is needed, roughly, to prove that the equation  $U(\beta) = 0$  has a consistent root  $\widehat{\beta}$ .

Ignoring higher order terms in a Taylor expansion will give

$$V(\beta)(\widehat{\beta} - \beta) \approx U(\beta)$$

where V = -U'. In the mle case we had identities relating the expectation of V to the variance of U. In general here we have

$$Var(U) = \sum x_i^2 Var(Y_i).$$

If  $Y_i$  is Poisson with mean  $\mu_i$  (and so  $Var(Y_i) = \mu_i$ ) this is

$$Var(U) = \sum x_i^2 \mu_i.$$

Moreover we have

$$V_i = x_i^2 \mu_i$$

and so

$$V(\beta) = \sum x_i^2 \mu_i \,.$$

The central limit theorem (the Lyapunov kind) will show that  $U(\beta)$  has an approximate normal distribution with variance  $\sigma_U^2 = \sum x_i^2 \text{Var}(Y_i)$  and so

$$\widehat{\beta} - \beta \approx N(0, \sigma_U^2 / (\sum x_i^2 \mu_i)^2)$$

If  $Var(Y_i) = \mu_i$ , as it is for the Poisson case, the asymptotic variance simplifies to  $1/\sum x_i^2 \mu_i$ .

Other estimating equations are possible, popular. If  $w_i$  is any set of deterministic weights (possibly depending on  $\mu_i$ ) then could define

$$U(\beta) = \sum w_i (Y_i - \mu_i)$$

and still conclude that U=0 probably has a consistent root which has an asymptotic normal distribution.

Idea widely used:

Example: Generalized Estimating Equations, Zeger and Liang.

Abbreviation: GEE.

Called by econometricians Generalized Method of Moments.

An estimating equation is unbiased if

$$E_{\theta}(U(\theta)) = 0$$

**Theorem**: Suppose  $\hat{\theta}$  is a consistent root of the unbiased estimating equation

$$U(\theta) = 0.$$

Let V = -U'. Suppose there is a sequence of constants  $B(\theta)$  such that

$$V(\theta)/B(\theta) \to 1$$

and let

$$A(\theta) = Var_{\theta}(U(\theta))$$

and

$$C(\theta) = B(\theta)A^{-1}(\theta)B(\theta).$$

Then

$$\sqrt{C(\theta_0)}(\widehat{\theta} - \theta_0) \Rightarrow N(0, 1)$$
$$\sqrt{C(\widehat{\theta})}(\widehat{\theta} - \theta_0) \Rightarrow N(0, 1)$$

Other ways to estimate A, B and C lead to same conclusions. There are multivariate extensions using matrix square roots.