Lecture 4:

Parametric Inference – continued

#### **Outline:**

- 1. MLE Optimality
- 2. The Delta Method
- 3. Multiparameter models
- 4. Parametric Bootstrap
- 5. Sufficient Statistics
- 6. Exponential Families
- 7. Computing MLE \*

<sup>\*</sup> covered in detail on the seminar

## **MLE Optimality**

- We already saw that MLE is asymptotically normal. But how does it compare (asymptotically) to other reasonable estimators?
- **Example**:  $X_1,...,X_n\sim \mathcal{N}(\theta,\sigma)$ . The MLE for  $\theta$  is  $\widehat{\theta}_n=\overline{X}_n$  the sample mean. For it,

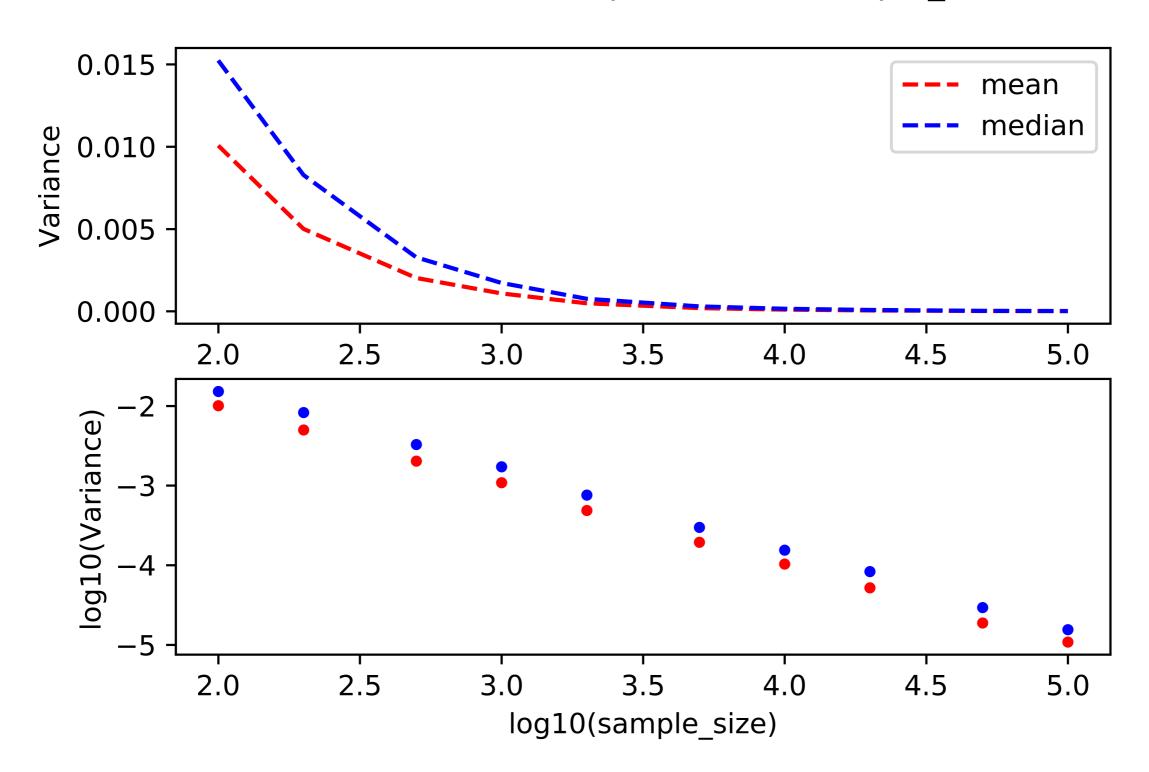
$$\sqrt{n}(\widehat{\theta}_n - \theta) \stackrel{P}{\to} \mathcal{N}(0, \sigma)$$

Another reasonable estimator for  $\theta$  is the sample median  $\hat{\theta}_n$ . For it we have

$$\sqrt{n}(\tilde{\theta}_n - \theta) \stackrel{P}{\to} \mathcal{N}(0, \sigma\sqrt{\pi/2})$$

## **MLE Optimality**

 $x \sim N(0, 1)$ , 1000 samples of size sample\_size



## **MLE Optimality**

• More generally, for two estimators  $T_n$  and  $U_n$  such that

$$\sqrt{n}(T_n-\theta) \overset{P}{\to} \mathcal{N}(0,\sigma=t) \text{ and } \sqrt{n}(U_n-\theta) \overset{P}{\to} \mathcal{N}(0,\sigma=u)$$

define **asymptotic relative efficiency** as  $ARE(U,T)=t^2/u^2$  – so in our normal example,  $ARE(\widetilde{\theta}_n,\widehat{\theta}_n)=2/\pi=0.63$  – median is 0.63 times as effective as mean (we are effectively using a fraction of the data).

• Theorem: If  $\widehat{\theta}_n$  is MLE and  $\widetilde{\theta}_n$  is any other estimator, then

$$\mathsf{ARE}(\widetilde{\theta}_n,\,\widehat{\theta}_n) \leq 1$$

so MLE is efficient or asymptotically optimal!

## The Delta Method

#### The Delta method

- Let  $\tau = g(\theta)$ , where g is a smooth function. The MLE of  $\tau$  is  $\widehat{\tau} = g(\widehat{\theta})$  (equivariance). But what is **the distribution** of  $\widehat{\tau}$ ?
- **Theorem** (The Delta method): If  $\tau = g(\theta)$  where g is diff. and  $g'(\theta) \neq 0$ , then

$$\begin{split} (\widehat{\boldsymbol{\tau}}_n - \boldsymbol{\tau}) / \hat{\operatorname{se}}(\widehat{\boldsymbol{\tau}}) & \xrightarrow{P} \mathcal{N}(0, 1) \quad \text{where } \widehat{\boldsymbol{\tau}}_n = g(\widehat{\boldsymbol{\theta}}_n) \quad \text{and} \\ \widehat{\operatorname{se}}(\widehat{\boldsymbol{\tau}}_n) &= |g'(\widehat{\boldsymbol{\theta}})| \, \hat{\operatorname{se}}(\widehat{\boldsymbol{\theta}}_n) \end{split}$$

This allows to build a  $(1 - \alpha)$ -confidence interval:

$$C_n = (\widehat{\tau}_n - z_{\alpha/2} \widehat{\text{se}}(\widehat{\tau}_n), \widehat{\tau}_n + z_{\alpha/2} \widehat{\text{se}}(\widehat{\tau}_n))$$

#### The Delta method

• Example: Let  $X_1, \ldots, X_n \sim \text{Bernoulli}(p)$  and let  $\psi = g(p) = \log \left( p/(1-p) \right)$ . The Fisher information is  $I(p) = 1/\left( p(1-p) \right)$ , so the estimated s.e. of the MLE  $\widehat{p}_n$  is

$$\widehat{\text{se}} = \sqrt{\frac{\widehat{p}_n(1-\widehat{p}_n)}{n}}. \quad \text{The MLE of } \psi \text{ is } \widehat{\psi} = \log \ \widehat{p}/(1-\widehat{p}).$$

Since g'(p) = 1/(p(1-p)), so

$$\widehat{\operatorname{se}}(\widehat{\psi}_n) = |g'(\widehat{p}_n)| \widehat{\operatorname{se}}(\widehat{p}_n) = \frac{1}{\sqrt{n\widehat{p}_n(1-\widehat{p}_n)}}$$

#### The Delta method

• Example: Recall that  $\hat{\operatorname{se}}(\hat{\theta}_n) = 1/\sqrt{I_n(\theta)}$  – Fisher information. Now let  $X_1, \ldots, X_n \sim \mathcal{N}(\mu, \sigma) - \mu$  is known and we want to estimate  $\psi = \log \sigma$ . Fisher info is **minus** the expectation of:

$$\frac{\partial^2 \log f(X; \sigma)}{\partial \sigma^2} = \frac{\partial^2}{\partial \sigma^2} \left( \log \sigma - \frac{(X - \mu)^2}{2\sigma^2} \right) = \frac{1}{\sigma^2} - \frac{3(X - \mu)^2}{\sigma^4}$$

so  $I(\sigma)=2/\sigma^2$ ,  $I_n(\sigma)=n\,I(\sigma)$  and  $\hat{\operatorname{se}}(\hat{\sigma}_n)=\hat{\sigma}_n/\sqrt{2n}$  and so for  $\psi=g(\sigma)=\log\sigma$  with  $g'=1/\sigma$  we have:

$$\widehat{\text{se}}(\widehat{\psi}_n) = \frac{1}{\widehat{\sigma}_n} \frac{\widehat{\sigma}_n}{\sqrt{2n}} = \frac{1}{\sqrt{2n}}$$

• Our ideas can be directly extended to models with several parameters.  $\theta = (\theta_1, ..., \theta_k)$  and MLE is  $\widehat{\theta} = (\widehat{\theta}_1, ..., \widehat{\theta}_k)$ . The matrix of minus expectations of second derivatives:

$$H_{ij} = \frac{\partial^2 \mathcal{C}_n}{\partial \theta_i \, \partial \theta_j} \quad \text{is} \quad \left( I_n(\theta) \right)_{ij} = - \, \mathbb{E}_{\theta}(H_{ij})$$

- called the Fisher information matrix.

It is handy to denote the **inverse of it**  $J_n(\theta) = I_n^{-1}(\theta)$ .

Theorem: Under appropriate regularity conditions,

$$(\widehat{\theta} - \theta) \approx \mathcal{N}(0, \Sigma = J_n)$$

and for  $\theta_{j}$  – j-th component of  $\theta$ 

$$\frac{\widehat{\theta}_j - \theta_j}{\widehat{\text{se}}_j} \overset{P}{\to} \mathcal{N}(0,1) \quad \text{where } \widehat{\text{se}}_j^2 = J_n(j,j) \text{ is the j-th diagonal}$$

element of  $J_n$ .

And the approximate covariance  ${\rm Cov}(\widehat{\theta}_j,\,\widehat{\theta}_k)\approx J_n(j,k)$  is the (j,k)-th non-diagonal element

• Theorem (Multiparameter Delta method): For  $\tau = g(\theta_1, ..., \theta_k)$ ,

denote 
$$\nabla g = \left(\frac{\partial g}{\partial \theta_1}, ..., \frac{\partial g}{\partial \theta_k}\right)^T$$
 the **gradient** of  $g$ . If  $\nabla g$ 

evaluated at  $\widehat{\theta}$ ,  $\widehat{\nabla g}$ , is not zero, for  $\widehat{\tau}=g(\widehat{\theta})$  we have

$$\frac{\widehat{\tau} - \tau}{\widehat{\text{se}}(\widehat{\tau})} \xrightarrow{P} \mathcal{N}(0,1) \text{ where}$$

$$\widehat{\operatorname{se}}(\widehat{\tau}) = \sqrt{(\widehat{\nabla g})^T \widehat{J}_n(\widehat{\nabla g})} \text{ where } \widehat{J}_n = J_n(\widehat{\theta}_n).$$

• Example.  $X_1, ..., X_n \sim \mathcal{N}(\mu, \sigma)$  and  $\tau = g(\mu, \sigma) = \sigma/\mu$ . We have

$$I_n(\mu,\sigma) = \frac{n}{\sigma^2} \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} \text{ hence } J_n = I_n^{-1} = \frac{\sigma^2}{2n} \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}$$

the gradient of g is  $\nabla g = \left(-\sigma/\mu^2, 1/\mu\right)^T$ 

thus 
$$\widehat{\text{se}}(\widehat{\tau}) = \sqrt{(\widehat{\nabla g})^T \widehat{J}_n(\widehat{\nabla g})} = \sqrt{\frac{1}{n\widehat{\mu}^4} + \frac{\widehat{\sigma}^2}{2\widehat{\mu}^2}}$$

## Parametric Bootstrap

#### Parametric Bootstrap

- We've introduced bootstrap in the **non-parametric** setting we sampled  $X_1^*, \ldots, X_n^*$  from the empirical CDF  $\widehat{F}_n$ . How does one extend it for parametric models? (To estimate standard errors and thus confidence intervals)
- Quite straightforward! We should sample  $X \sim f(x; \widehat{\theta}_n)$  where  $\widehat{\theta}_n$  is either MLE or MOM-estimator.
- See an example on the next slide

### Parametric Bootstrap

- **Example**: Recall estimating  $\tau = \sigma/\mu$  for the normal distribution. To do parametric bootstrap:
- **1.** Simulate (sample)  $X_1^*, ..., X_n^* \sim \mathcal{N}(\widehat{\mu}, \widehat{\sigma})$
- **2.** Compute  $\hat{\mu}^* = n^{-1} \sum_i X_i^*$  and  $(\hat{\sigma}^*)^2 = n^{-1} \sum_i (X_i^* \hat{\mu}^*)^2$
- **3.** Compute  $\hat{\tau}^* = g(\hat{\mu}^*, \hat{\sigma}^*) = \hat{\sigma}^*/\hat{\mu}^*$
- **4.** Repeating this B times gives  $\hat{\tau}_1^*, ..., \hat{\tau}_B^*$

From that bootstrap sample, get the std! This is simpler than the Delta method, but the latter gives an analytic expression.

- A **statistic** is a function  $T(X^n)$  of the data.
- **Definition**: Write  $x^n \leftrightarrow y^n$  if  $f(x^n; \theta) = cf(y^n; \theta)$  for some constant c that might depend on  $x^n$  and  $y^n$  but not  $\theta$ . A statistic  $T(x^n)$  is **sufficient** if  $T(x^n) \leftrightarrow T(y^n)$  implies  $x^n \leftrightarrow y^n$ .
- So if  $x^n \leftrightarrow y^n$ , then the likelihood function based on  $x^n$  has the same shape as the likelihood function based on  $y^n$ . Roughly, a statistic  $T(X^n)$  is sufficient if we can calculate the likelihood knowing only  $T(X^n)$ .
- Example:  $X_1, ..., X_n \sim \text{Bernoulli}(p)$ . Then  $\mathcal{L}(p) = p^S (1-p)^{n-S}$  where  $S = \sum X_i$ . So S is sufficient

• **Example**: Let  $X_1, ..., X_n \sim \mathcal{N}(\mu, \sigma)$  and let  $T = (\overline{X}, S)$ . Then

$$f(X^n; \mu, \sigma) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^n \exp\left\{-\frac{nS^2}{2\sigma^2}\right\} \exp\left\{-\frac{n(\bar{X} - \mu)^2}{2\sigma^2}\right\}$$

where  $S^2$  is sample variance. So  $T=(\overline{X},S)$  is a sufficient statistic, as well as  $U=(2\overline{X},S-1)$  is. These are sufficient as well:  $T_1(X^n)=(X_1,\ldots,X_n),\,T_2(X^n)=(\overline{X},S),\,T_3(X^n)=\overline{X}$  is not.  $T_4(X^n)=(\overline{X},S,X_3)$  is. Notice that  $T_2$  is a function of  $T_1,\,T_2$  is a function of  $T_4$ .

Definition: A statistic is minimal sufficient if 1) it is sufficient, and
2) it is a function of every other sufficient statistic

- So for  $\mathcal{N}(\mu,\sigma)$ ,  $T=(\overline{X},S)$  is a minimal sufficient statistic. For Bernoulli,  $T=\sum X_i$  is. For Poisson,  $T=\sum X_i$  as well.
- **Exercise**: Let  $(X_1, X_2) \sim \text{Bernoulli}(p)$ . Figure out that  $T = X_1 + X_2$  is sufficient statistic.
- **Theorem** (Factorization): T is sufficient if and only if there are functions  $g(t,\theta)$  and h(x) such that  $f(x^n;\theta) = g(t(x^n),\theta) h(x^n)$
- **Example**: For the above exercise,  $t = x_1 + x_2$

$$f(x_1, x_2; \theta) = f(x_1; \theta) f(x_2; \theta) = \theta^{x_1} (1 - \theta)^{1 - x_1} \theta^{x_2} (1 - \theta)^{1 - x_2} = g(t, \theta) h(x_1, x_2)$$
  
where  $g(t, \theta) = \theta^t (1 - \theta)^{2 - t}$  and  $h(x_1, x_2) = 1$ .

- Why bother with sufficient statistics? Let  $\widehat{\theta}$  be an estimator of  $\theta$ . The Rao-Blackwell theorem says that **an estimator should only depend on the sufficient statistic**, otherwise it can be improved! Denote  $R(\theta, \widehat{\theta}) = \mathbb{E}_{\theta}(\theta \widehat{\theta})^2$  the MSE of the estimator.
- Theorem (Rao-Blackwell): Let  $\widehat{\theta}$  be an estimator and let T be a sufficient statistic. Define a new estimator by

$$\tilde{\theta} = \mathbb{E}_{\theta}(\hat{\theta} \mid T)$$

then, for any  $\theta$ , it holds that  $R(\theta, \tilde{\theta}) \leq R(\theta, \hat{\theta})$ !

• Most of parametric models we studied so far are special cases of a general class of models called **exponential families**. We say that  $\{f(x;\theta):\theta\in\Theta\}$  is a one-parameter exponential family if there are functions  $\eta(\theta),\,B(\theta),\,T(x)$  and h(x) such that

$$f(x; \theta) = h(x) e^{\eta(\theta)T(x) - B(\theta)}$$

such T(x) is called the **natural sufficient statistic**.

• Example:  $X \sim \operatorname{Poisson}(\theta)$ . Then  $f(x;\theta) = \frac{\theta^x e^{-\theta}}{x!} = \frac{1}{x!} e^{x \log \theta - \theta}$  so  $\eta(\theta) = \log \theta$ ,  $B(\theta) = \theta$ , T(x) = x and h(x) = 1/(x!)

• **Example**:  $X \sim \text{Binomial}(n, \theta)$ . Then

$$f(x;\theta) = \binom{n}{x} \theta^{x} (1-\theta)^{n-x} = \binom{n}{x} \exp\left\{x \log\left(\frac{\theta}{1-\theta}\right) + n\log(1-\theta)\right\}$$

so in this case  $\eta(\theta) = \log(\theta/(1-\theta))$ ,  $B(\theta) = -n\log\theta$  and

$$T(x) = x, \ h(x) = \binom{n}{x}.$$

• An exponential family can be rewritten as  $f(x;\eta) = h(x)\,e^{\eta T(x) - A(\eta)} \text{ where } \eta = \eta(\theta) \text{ is called the } \mathbf{natural}$   $\mathbf{parameter} \text{ and } A(\eta) = \log \left[ h(x)\,e^{\eta T(x)} dx \right]$ 

• For example, Poisson  $f(x; \eta) = e^{\eta x - e^{\eta}}/x!$  and  $\eta = \log \theta$ .

Theorem: For X with density from exp. family,

$$\mathbb{E}(T(X)) = A'(\eta) \text{ and } \mathbb{V}(T(X)) = A''(\eta)$$

• If  $\theta = (\theta_1, ..., \theta_k)$  is a vector, then

$$f(x;\theta) = h(x) \exp\left\{\sum_{j=1}^{k} \eta_j(\theta) T_j(x) - B(\theta)\right\} \text{ where }$$

 $T=(T_1,\ldots,T_k)$  is the sufficient statistic. IID sample of size n also has sufficient statistic (  $\sum_i T_1(X_i),\ldots,\sum_i T_k(X_i)$ ). Then also

$$\mathbb{E}(T(X)) = A'(\eta)$$
 (a vector) and  $\mathbb{V}(T(X)) = A''(\eta)$  (a matrix)

# **Computing MLE**

## **Computing MLE**

- This is all good, but we only have analytic formulae for MLE for the simplest models – for the whole exponential family, but still – if a model is more complicated than that, we need **numerical methods** already.
- On the seminar, we'll cover:
  - 1. The Newton-Raphson method
  - 2. The Expectation Maximization (EM) Algoritm

## **Computing MLE**

Motivation: Mixture of 2 normal distributions:

