#### **Likelihood Inference**

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### Likelihood Function and MLE

- Joint distribution:  $(Y_1, \ldots, Y_n) \sim f(Y_1, \ldots, Y_n \mid \theta)$  where  $\theta \in \Theta$
- Idea: Choose the estimate of  $\theta$  such that the likelihood of obtaining the sample you actually obtained is maximized
- Likelihood function:  $L(\theta \mid Y_1, ..., Y_n) = f(Y_i, ..., Y_n \mid \theta)$
- Log-likelihood function:  $I(\theta \mid Y_1, ..., Y_n) \equiv \log L(\theta \mid Y_1, ..., Y_n)$
- Function of  $\theta$  given the data
- Likelihood Principle: If Y and  $\widetilde{Y}$  are two samples and  $L(\theta \mid Y) \propto L(\theta \mid \widetilde{Y})$ , then inferences about  $\theta$  one would draw from Y and  $\widetilde{Y}$  are the same
- Maximum likelihood estimation (MLE):

$$\hat{\theta}_n \equiv \underset{\theta \in \Theta}{\operatorname{argmax}} L(\theta \mid Y_1, \dots, Y_n) = \underset{\theta \in \Theta}{\operatorname{argmax}} I(\theta \mid Y_1, \dots, Y_n)$$

## Normal Regression Model

- Model:  $Y_i \mid X_i \stackrel{\text{indep.}}{\sim} \mathcal{N}(X_i^{\top}\beta, \sigma^2)$
- Or equivalently:  $Y_i = X_i^{\top} \beta + \epsilon_i$  where  $\epsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2)$
- Likelihood and log-likelihood functions:

$$L_{n}(\beta, \sigma^{2} \mid Y, \mathbf{X}) = (2\pi\sigma^{2})^{-n/2} \exp\left\{-\frac{1}{2\sigma^{2}} \sum_{i=1}^{n} (Y_{i} - X_{i}^{\top}\beta)^{2}\right\}$$

$$I_{n}(\beta, \sigma^{2} \mid Y, \mathbf{X}) = -\frac{n}{2} \log 2\pi - \frac{n}{2} \log \sigma^{2} - \frac{1}{2\sigma^{2}} \sum_{i=1}^{n} (Y_{i} - X_{i}^{\top}\beta)^{2}$$

 Solving the first order condition (and checking the second order condition) yields the following MLE:

$$\hat{\beta} = \left(\sum_{i=1}^{n} X_i X_i^{\top}\right)^{-1} \sum_{i=1}^{n} X_i Y_i, \text{ and } \hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^{n} (Y_i - X_i^{\top} \hat{\beta})^2$$

## Consistency

- $\theta_0$ : True value of  $\theta$
- $\hat{\theta}_n$ : MLE of  $\theta$  as a function of sample size
- Theorem: If  $Y_1, \ldots, Y_n \overset{\text{i.i.d.}}{\sim} f(Y_i \mid \theta_0)$ , then  $\hat{\theta}_n \equiv \operatorname{argmax}_{\theta \in \Theta} I_n(\theta \mid Y) \overset{P}{\longrightarrow} \theta_0$  under some regularity conditions
- Identification: the maximum value of  $L(\theta \mid Y)$  exists and is unique

## Intuitive "proof"

- Show  $\hat{\theta}_n \stackrel{P}{\longrightarrow} \hat{\theta} \equiv \operatorname{argmax}_{\theta \in \Theta} \mathbb{E} \{ \log f(Y_i \mid \theta) \}$
- Recall Jensen's inequality: For any concave (convex) function  $g(\cdot)$  and a random variable X, we have  $\mathbb{E}\{g(X)\} \leq g(\mathbb{E}(X))$  ( $\mathbb{E}\{g(X)\} \geq g(\mathbb{E}(X))$ )
- Show that Kullback-Leibler Divergence is non-negative, i.e.,

$$\mathbb{E}(\log f(Y_i \mid \theta_0) - \log f(Y_i \mid \hat{\theta})) \geq 0$$

• Argue that the equality holds if and only if  $\hat{\theta} = \theta_0$ 

### Score and Fisher Information

Score statistic:

$$s_n(\tilde{\theta}) \equiv \frac{\partial}{\partial \theta} I_n(\theta \mid Y) \Big|_{\theta = \tilde{\theta}}$$

Mean of score is zero:

$$\mathbb{E}(s_{i}(\theta_{0})) = \int \frac{\partial}{\partial \theta} I(\theta \mid Y_{i}) \Big|_{\theta=\theta_{0}} f(Y_{i} \mid \theta_{0}) dY_{i}$$
$$= \int \frac{\partial}{\partial \theta} f(Y_{i} \mid \theta) \Big|_{\theta=\theta_{0}} dY_{i} = 0$$

Fisher information:

$$\Omega(\theta_0) \equiv \mathbb{E}(s_i(\theta_0)s_i(\theta_0)^{\top}) = \mathbb{V}(s_i(\theta_0))$$

## Information Equality

Information Equality:

$$\mathbb{E}(\mathbf{H}_i(\theta_0)) = -\Omega(\theta_0)$$

where the Hessian matrix is given by,

$$\mathbf{H}_{n}(\tilde{\theta}) \equiv \frac{\partial^{2}}{\partial \theta \partial \theta^{\top}} I_{n}(\theta \mid Y) \Big|_{\theta = \tilde{\theta}}$$

- Proof:
  - Using the basic rules of calculus, show

$$\mathbb{E}(s_i(\theta_0)s_i(\theta_0)^{\top}) = \int \frac{\partial^2}{\partial\theta\partial\theta^{\top}} f(Y_i \mid \theta) \Big|_{\theta=\theta_0} dY_i - \mathbb{E}(s_i(\theta_0)s_i(\theta_0)^{\top})$$

Show that the first term in the above equation is zero

## **Asymptotic Normality**

• Taylor expansion around  $\theta_0$ :

$$0 = s_n(\hat{ heta}_n) pprox s_n( heta_0) + \mathsf{H}_n( heta_0)(\hat{ heta}_n - heta_0)$$

Asymptotic distribution:

$$\sqrt{n}(\hat{\theta}_{n} - \theta_{0}) \approx \underbrace{\left(-\frac{1}{n} \sum_{i=1}^{n} \mathbf{H}_{i}(\theta_{0})\right)^{-1}}_{\stackrel{P}{\longrightarrow} \Omega(\theta_{0})^{-1}} \underbrace{\sqrt{n} \left(\frac{1}{n} \sum_{i=1}^{n} s_{i}(\theta_{0})\right)}_{\stackrel{D}{\longrightarrow} \mathcal{N}(0, \Omega(\theta_{0}))}$$

$$\stackrel{D}{\longrightarrow} \mathcal{N}\left(0, \Omega(\theta_{0})^{-1}\right)$$

- Approximate variance:  $\mathbb{V}(\hat{\theta}_n) \approx \frac{1}{n}\Omega(\theta_0)^{-1}$
- Variance estimator:  $\widehat{\mathbb{V}(\hat{\theta}_n)} = -\mathbf{H}_n(\hat{\theta}_n)^{-1}$

# Normal Regression Model, Again

- Parameters:  $\theta = (\beta, \sigma^2)$
- Score statistic:

$$s_n(\theta_0) = \begin{bmatrix} \frac{1}{\sigma^2} X^{\top} (Y - \mathbf{X}\beta) \\ -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} ||Y - \mathbf{X}\beta||^2 \end{bmatrix}$$

Hessian matrix:

$$\mathbf{H}_{n}(\theta_{0}) = \begin{bmatrix} -\frac{1}{\sigma^{2}}\mathbf{X}^{\top}\mathbf{X} & -\frac{1}{\sigma^{4}}\mathbf{X}^{\top}(Y - \mathbf{X}\beta) \\ -\frac{1}{\sigma^{4}}(Y - \mathbf{X}\beta)^{\top}\mathbf{X} & \frac{n}{2\sigma^{4}} - \frac{1}{\sigma^{6}}\|Y - \mathbf{X}\beta\|^{2} \end{bmatrix}$$

• Information matrix:

$$\Omega(\theta_0) = \mathbb{E}(s_i(\theta_0)s_i(\theta_0)^\top \mid \mathbf{X}) = -\mathbb{E}\left(\frac{\mathbf{H}_n(\theta_0)}{n}\middle| \mathbf{X}\right) = \begin{bmatrix} \frac{1}{n\sigma^2}\mathbf{X}^\top\mathbf{X} & 0\\ 0 & \frac{1}{2\sigma^4} \end{bmatrix}$$

Approximate variance:

$$\mathbb{V}(\hat{\theta}_n \mid \mathbf{X}) \approx \begin{bmatrix} \sigma^2 (\mathbf{X}^\top \mathbf{X})^{-1} & 0 \\ 0 & \frac{2\sigma^4}{n} \end{bmatrix}$$

### Invariance and Transformation

- If  $\hat{\theta}_n$  is the MLE of  $\theta$ , the MLE of  $g(\theta)$  is  $g(\hat{\theta}_n)$  for any function  $g(\cdot)$
- But, to improve the asymptotic normal approximation of the sampling distribution, we can use transformations
  - $\bullet \in (0,\infty) \longrightarrow \log \theta$
  - 2  $\theta \in (0,1) \longrightarrow \log\left(\frac{\theta}{1-\theta}\right)$  logistic
- In normal regression, let's change  $\sigma^2$  to  $\gamma \equiv \log \sigma^2$ . Then,

$$\frac{\partial}{\partial \gamma} I_n(\beta, \gamma \mid Y, \mathbf{X}) = \frac{\partial \sigma^2}{\partial \gamma} \frac{\partial}{\partial \sigma^2} I_n(\beta, \sigma^2 \mid Y, \mathbf{X})$$

$$= -\exp(\gamma) \left\{ \frac{n}{2 \exp(\gamma)} - \frac{1}{2 \exp(2\gamma)} \|Y - \mathbf{X}\beta\|^2 \right\}$$

## **Asymptotic Efficiency**

• Cramer-Rao Inequality: Let  $\tilde{\theta}_n$  be any estimator.

$$\mathbb{V}(\tilde{\theta}_n) \geq \frac{\partial}{\partial \theta_0} \mathbb{E}(\tilde{\theta}_n) \left\{ n \mathbb{E}(s_i(\theta_0) s_i(\theta_0)^\top) \right\}^{-1} \left\{ \frac{\partial}{\partial \theta_0} \mathbb{E}(\tilde{\theta}_n) \right\}^\top$$

where 
$$\mathbb{E}(\tilde{\theta}_n) = \int \tilde{\theta}_n f(Y \mid \theta_0) dY$$

ullet For any asymptotically unbiased estimator  $\tilde{\theta}_n$ , we have

$$\mathbb{V}(\tilde{\theta}_n) \geq \frac{1}{n}\Omega(\theta_0)^{-1}$$

- MLE achieves the Cramer-Rao Lower Bound for any  $\theta_0$
- MLE is asymptotically uniformly minimum variance unbiased estimator (UMVUE)

### **Outline of Proof**

Show

$$\frac{\partial}{\partial \theta_0} \mathbb{E}(\tilde{\theta}_n) \; = \; \mathbb{E}\left\{\tilde{\theta}_n \frac{\partial}{\partial \theta_0} \log f(Y \mid \theta_0)\right\}$$

Show

$$\operatorname{Cov}\left(\tilde{\theta}_n, \ \frac{\partial}{\partial \theta_0} \log f(Y \mid \theta_0)\right) \ = \ \frac{\partial}{\partial \theta_0} \mathbb{E}(\tilde{\theta}_n)$$

By the Covariance inequality,

$$\left| \frac{\partial}{\partial \theta_0} \mathbb{E}(\tilde{\theta}_n) \left\{ \frac{\partial}{\partial \theta_0} \mathbb{E}(\tilde{\theta}_n) \right\}^{\top} \right| \leq \left| \mathbb{V}(\tilde{\theta}_n) \mathbb{V} \left\{ \frac{\partial}{\partial \theta_0} \log f(Y \mid \theta_0) \right\} \right|$$

## **Model Misspecification**

- What happens if the model is wrong?
- True model:  $Y_i \stackrel{\text{i.i.d.}}{\sim} g(Y_i)$
- Misspecified model:  $Y_i \stackrel{\text{i.i.d.}}{\sim} f(Y_i \mid \theta_0)$
- $\hat{\theta}_n \stackrel{P}{\longrightarrow} \theta_0$  such that

$$\theta_0 = \underset{\theta \in \Theta}{\operatorname{argmin}} \underbrace{\int \log \frac{g(Y_i)}{f(Y_i \mid \theta)} g(Y_i) \, dY_i}_{\textit{Kullback-Leibler divergence}}$$

Asymptotic distribution:

$$\sqrt{n}(\hat{\theta}_n - \theta_0) \stackrel{D}{\longrightarrow} \mathcal{N}\left(0, \ \mathbb{E}(-\mathbf{H}_i(\theta_0))^{-1}\mathbb{E}(s_i(\theta_0)s_i(\theta_0)^\top)\mathbb{E}(-\mathbf{H}_i(\theta_0))^{-1}\right)$$

Information equality does not hold

### Robust Standard Error

Sandwich estimator:

bread = 
$$\left(-\frac{1}{n}\mathbf{H}_n(\hat{\theta}_n)\right)^{-1}$$
, and meat =  $\frac{1}{n}\sum_{i=1}^n \mathbf{s}_i(\hat{\theta}_n)\mathbf{s}_i(\hat{\theta}_n)^{\top}$ 

- Clustering: a wrong likelihood function
- Cluster robust standard error:

meat = 
$$\frac{1}{n} \sum_{g=1}^{G} \left\{ \left( \sum_{i=1}^{n_g} s_i(\hat{\theta}_n) \right) \left( \sum_{i=1}^{n_g} s_i(\hat{\theta}_n) \right)^{\top} \right\}$$

• "Correct" standard error for "wrong" estimate

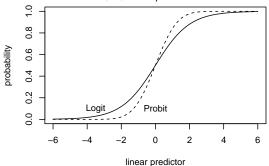
### Logit and Probit Models

• Logit model for binary outcome  $Y_i \in \{0, 1\}$ :

$$Y_i \overset{\text{indep.}}{\sim} \operatorname{Bernoulli}(\pi_i)$$

$$\pi_i = \frac{\exp(X_i^{\top}\beta)}{1 + \exp(X_i^{\top}\beta)} = \frac{1}{1 + \exp(-X_i^{\top}\beta)}$$

- Logit:  $logit(\pi_i) \equiv log(\pi_i/(1-\pi_i)) = X_i^{\top}\beta$
- Probit:  $\Phi^{-1}(\pi_i) = X_i^{\top} \beta$



- monotone increasing
- symmetric around 0
- maximum slope at 0
- logit coef. = probit coef ×1.6

## Latent Variable Interpretation

- The latent variable or the "Utility":  $Y_i^*$
- The Model:

$$Y_{i} = \begin{cases} 1 & \text{if } Y_{i}^{*} > 0 \\ 0 & \text{if } Y_{i}^{*} \leq 0 \end{cases}$$

$$Y_{i}^{*} = X_{i}^{\top} \beta + \epsilon_{i} \quad \text{with} \quad \mathbb{E}(\epsilon_{i}) = 0$$

- Logit:  $\epsilon_i \stackrel{\text{i.i.d.}}{\sim} \text{logistic}$  (the density is  $\exp(-\epsilon_i)/\{1 + \exp(-\epsilon_i)\}^2$ )
- Probit:  $\epsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0,1)$
- The variance of  $Y_i^*$  is not identifiable
- The "cutpoint" is not identifiable

### Inference with the Logit and Probit Models

Likelihood and log-likelihood functions:

$$L_n(\beta \mid Y, \mathbf{X}) = \prod_{i=1}^n \pi_i^{Y_i} (1 - \pi_i)^{1 - Y_i}$$

$$I_n(\beta \mid Y, \mathbf{X}) = \sum_{i=1}^n \{ Y_i \log \pi_i + (1 - Y_i) \log (1 - \pi_i) \}$$

- Logit model:

  - Score function:  $s_n(\beta) = \sum_{i=1}^n (Y_i \pi_i) X_i$  Hessian:  $\mathbf{H}_n(\beta) = -\sum_{i=1}^n \pi_i (1 \pi_i) X_i X_i^\top \le 0$
  - Approximate variance:  $\mathbb{V}(\hat{\beta}_n \mid \mathbf{X}) \approx \{\sum_{i=1}^n \pi_i (1 \pi_i) X_i X_i^\top\}^{-1}$
  - Globally concave

## Newton-Raphson Algorithm

- Find  $\hat{\theta}_n$  such that  $s_n(\hat{\theta}_n) = 0$
- Mean Value Theorem: If f(x) is continuous and differentiable on [a, b], then there exists  $c \in [a, b]$  such that

$$\frac{\partial}{\partial x}f(x)\Big|_{x=c}=\frac{f(b)-f(a)}{b-a}$$

ullet Thus, for  $ilde{ heta} \in [ heta^{(t)}, \hat{ heta}_n]$ ,

$$s_n(\theta^{(t)}) = s_n(\theta^{(t)}) - s_n(\hat{\theta}_n) = \mathbf{H}_n(\tilde{\theta})(\theta^{(t)} - \hat{\theta}_n)$$

• The algorithm: converges at  $\hat{\theta}_n$ 

$$\theta^{(t+1)} = \theta^{(t)} - \mathbf{H}_n(\theta^{(t)})^{-1} s_n(\theta^{(t)})$$

- Fisher scoring algorithm: use  $\Omega(\theta^{(t)})^{-1}$  (always positive-definite)
- Global maxima vs. local maxima: different starting values

## Calculating Quantities of Interest

Logistic regression coefficients are NOT quantities of interest

• Predicted probability: 
$$\pi(x) = \Pr(Y = 1 \mid X = x) = \frac{\exp(x^{\top}\beta)}{1 + \exp(x^{\top}\beta)}$$

- Attributable risk (risk difference):  $\pi(x_1) \pi(x_0)$
- Relative risk:  $\pi(x_1)/\pi(x_0)$
- Odds and odds ratio:  $\frac{\pi(x)}{1-\pi(x)}$  and  $\frac{\pi(x_1)/\{1-\pi(x_1)\}}{\pi(x_0)/\{1-\pi(x_0)\}}$
- Average Treatment Effect:

$$\mathbb{E}\{\Pr(Y_i = 1 \mid T_i = 1, X_i) - \Pr(Y_i = 1 \mid T_i = 0, X_i)\}$$

- MLE: plug in  $\hat{\beta}_n$
- Asymptotic distribution: the Delta method (a bit painful!)

$$\sqrt{n}(\hat{\pi}(x) - \pi(x)) \stackrel{D}{\longrightarrow} \mathcal{N}\left(0, \ \frac{\pi(x)^2}{\{1 + \exp(x^\top \beta_0)\}^2} x^\top \Omega(\beta_0)^{-1} x\right)$$

## "Bayesian" Monte Carlo Approximation

Bayesians: parameters are random variables

$$\underbrace{posterior}_{p(\theta \mid Y)} = \underbrace{\frac{p(Y \mid \theta)}{p(\theta)} p(\theta)}_{p(Y \mid \theta)p(\theta)d\theta} \propto p(Y \mid \theta)p(\theta)$$

$$\underbrace{\int p(Y \mid \theta)p(\theta)d\theta}_{p(\theta)d\theta} \propto p(Y \mid \theta)p(\theta)$$
marginal likelihood

- Bernstein Von Mises Theorem: For a large sample, Bayes estimate is close to the MLE. The posterior distribution of the parameter around the posterior mean is also close to the distribution of the MLE around the truth,
- Sample  $\theta$  from  $\mathcal{N}(\hat{\theta}_n, -\mathbf{H}_n(\hat{\theta}_n)^{-1})$  and compute "Bayes" estimate and confidence interval of  $g(\theta)$  for any function  $g(\cdot)$

### **Bootstrap**

- Unknown data generating process:  $Y_i \stackrel{\text{i.i.d.}}{\sim} F$
- Want to know  $\mathbb{V}_F(\hat{\theta}_n)$  where  $\theta_n \equiv g(Y_1, \dots, Y_n)$
- Approximate it with  $\mathbb{V}_{\widehat{F}_n}(\widehat{\theta}_n)$  where  $\widehat{F}_n$  is the empirical CDF
- Real world:  $F \Longrightarrow Y_1, \ldots, Y_n \Longrightarrow \hat{\theta}_n$
- Bootstrap world:  $\widehat{F}_n \Longrightarrow Y_1^*, \ldots, Y_n^* \Longrightarrow \widehat{\theta}_n^* \equiv g(Y_1^*, \ldots, Y_n^*)$

$$\hat{\sigma}_{boot}^2 \equiv \frac{1}{B} \sum_{b=1}^{B} \left( \hat{\theta}_{n,b}^* - \frac{1}{B} \sum_{b'=1}^{B} \hat{\theta}_{n,b'}^* \right)^2$$

Asymptotic approximation:

$$\mathbb{V}_{F}(\hat{\theta}_{n}) \overset{\textit{may not be so small}}{\approx} \mathbb{V}_{\widehat{F}_{n}}(\hat{\theta}_{n}) \overset{\textit{small}}{\approx} \hat{\sigma}_{\textit{boot}}^{2}$$

- Bootstrap percentile confidence intervals
- Parametric bootstrap: Replace  $\widehat{F}_n$  with  $F_{\widehat{\theta}_n}$

## Bootstrap and Estimation of Bias

- Real world:  $F \Longrightarrow Y_1, \ldots, Y_n \Longrightarrow \mathrm{bias}_F = \mathbb{E}_F(\hat{\theta}_n) \theta(F)$
- Bootstrap world:  $\widehat{F}_n \Longrightarrow Y_1^*, \dots, Y_n^* \Longrightarrow \operatorname{bias}_{\widehat{F}_n} = \mathbb{E}_{\widehat{F}_n}(\widehat{\theta}_n^*) \theta(\widehat{F}_n)$ where  $\theta(\widehat{F}_n) = \widehat{\theta}_n$  and  $\widehat{\mathbb{E}_{\widehat{F}_n}}(\widehat{\theta}_n^*) = \frac{1}{B} \sum_{b=1}^B \widehat{\theta}_{n,b}^*$
- Bootstrap percentile confidence interval: take 100  $\cdot$   $\alpha/2$  and 100  $\cdot$  (1  $\alpha/2$ ) percentiles
- bias corrected estimator:  $\hat{\theta}_n \widehat{\text{bias}} = 2\hat{\theta}_n \frac{1}{B} \sum_{b=1}^B \hat{\theta}_{n,b}^*$
- Bias-corrected confidence interval: see Efron and Tibshirani
- An example: Ratio estimator  $\hat{\theta}_n = \sum_{i=1}^n Y_i / \sum_{i=1}^n X_i$
- bias<sub>F</sub> =  $\mathbb{E}(\hat{\theta}_n) \mathbb{E}(Y_i)/\mathbb{E}(X_i) \neq 0$
- Computational note: resample indices, not data themselves

## Likelihood Ratio Test (LRT)

- Null hypothesis:  $H_0: \theta \in \Theta_0 \subset \Theta$  with  $H_1: \theta \in \Theta \setminus \Theta_0$
- "Nested" models:  $H_0: g_1(\theta) = \cdots = g_K(\theta) = 0$
- Unlike F test, nonlinear constraints are allowed
- Likelihood ratio statistic:

$$\lambda_{n}(Y) \equiv \underbrace{\frac{\displaystyle \sup_{\theta \in \Theta_{0}} L_{n}(\theta \mid Y)}{\sup_{\theta \in \Theta} L_{n}(\theta \mid Y)}}_{\textit{MLE}} = \frac{L_{n}(\bar{\theta}_{n} \mid Y)}{L_{n}(\hat{\theta}_{n} \mid Y)} \in (0, 1)$$

Asymptotic distribution:

$$-2\log \lambda_n(Y) \stackrel{D}{\longrightarrow} \chi_K^2$$

where  $K = dim(\Theta) - dim(\Theta_0)$ : the difference between the number of free parameters in  $\Theta$  and  $\Theta_0$ 

## Proof for a Special Case

- $H_0: \theta = \theta_0$  with  $H_1: \theta \neq \theta_0$
- Taylor expansion (again!):

$$I_n(\theta_0 \mid Y) \approx I_n(\hat{\theta}_n \mid Y) + s_n(\hat{\theta}_n \mid Y)(\hat{\theta}_n - \theta_0) + \frac{1}{2}(\hat{\theta}_n - \theta_0)^{\top} \mathbf{H}_n(\hat{\theta}_n)(\hat{\theta}_n - \theta_0)$$

Under the null hypothesis,

$$-2\log \lambda_{n}(Y) = -2\{I_{n}(\theta_{0} \mid Y) - I_{n}(\hat{\theta}_{n} \mid Y)\}$$

$$\approx \underbrace{\sqrt{n}(\hat{\theta}_{n} - \theta_{0})^{\top}}_{\underline{d} \mathcal{N}(0,\Omega(\theta_{0})^{-1})} \underbrace{-\frac{1}{n} \sum_{i=1}^{n} \mathbf{H}_{i}(\hat{\theta}_{n})}_{\underline{p} \mathcal{N}(\theta_{0})} \underbrace{\sqrt{n}(\hat{\theta}_{n} - \theta_{0})}_{\underline{d} \mathcal{N}(0,\Omega(\theta_{0})^{-1})}$$

$$\stackrel{d}{\longrightarrow} \chi_{K}^{2}$$

### Wald and Score Tests

- $H_0: g_1(\theta) = \cdots = g_K(\theta) = 0$
- Wald test: No need to calculate  $\bar{\theta}_n$

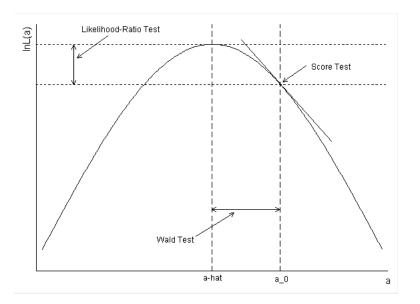
$$W_n \equiv ng(\hat{\theta}_n)^{\top} \{g^{(1)}(\hat{\theta}_n)^{\top} \Omega(\hat{\theta}_n)^{-1} g^{(1)}(\hat{\theta}_n)\}^{-1} g(\hat{\theta}_n) \stackrel{d}{\longrightarrow} \chi_K^2$$
  
$$\equiv -g(\hat{\theta}_n)^{\top} \{g^{(1)}(\hat{\theta}_n)^{\top} \mathbf{H}_n(\hat{\theta}_n)^{-1} g^{(1)}(\hat{\theta}_n)\}^{-1} g(\hat{\theta}_n) \stackrel{d}{\longrightarrow} \chi_K^2$$

• (Rao's) Score test: No need to calculate  $\hat{\theta}_n$ 

$$R_n \equiv -s_n(\bar{\theta}_n)^{\top} \mathbf{H}_n(\bar{\theta}_n)^{-1} s_n(\bar{\theta}_n) \stackrel{d}{\longrightarrow} \chi_K^2$$

- LRT requires the calculation of both  $\bar{\theta}_n$  and  $\hat{\theta}_n$
- But, they are all asymptotically equivalent!

## Geometry of Likelihood Ratio, Wald, and Score Tests



### Model Assessment, Selection, and Validation

- Likelihood ratio test works only for comparison of nested models
   what about non-nested models?
- In-sample (training) error vs. Out-of-sample (test) error  $\Longrightarrow \frac{1}{n} \sum_{i=1}^{n} L(Y_i, \hat{f}(X_i))$  vs.  $\mathbb{E}\{L(Y_i, \hat{f}(X_i))\}$
- Prediction error is measured with *loss function*  $L(\cdot, \cdot)$ 
  - classification error (0 1 loss):  $\mathbf{1}\{Y_i \neq \hat{f}(X_i)\}$
  - 2 squared error:  $(Y_i \hat{f}(X_i))^2$
  - **3** absolute error:  $|Y_i \hat{f}(X_i)|$
  - deviance: -2 · loglikelihood
- If you have a lot of data, you can randomly split the data into:
  - training data: fit the model
  - 2 validation data: estimate prediction error for model selection
  - test data: test the predictive performance of the final model
- But, we are usually not that fortunate...

### Bias and Variance Tradeoff

Recall the bias-variance decomposition:

$$\underbrace{\mathbb{E}\{(\hat{\theta} - \theta)^2\}}_{MSE} = \underbrace{\{\mathbb{E}(\hat{\theta} - \theta)\}^2}_{bias^2} + \underbrace{\mathbb{V}(\hat{\theta})}_{variance}$$

- Assume the model:  $Y_i = f(X_i) + \epsilon_i$  and  $\mathbb{E}(\epsilon_i) = 0$
- Expected prediction error at  $X_i$ :

$$\mathbb{E}\{(Y_i^{\mathsf{new}} - \hat{f}(X_i))^2\} \ = \ \{\mathbb{E}(\hat{f}(X_i) - f(X_i))\}^2 + \mathbb{V}(\hat{f}(X_i)) + \mathbb{V}(\epsilon_i)$$

- Making  $\hat{f}$  complex  $\Longrightarrow$  low bias, high variance
- Sample average prediction error (SAPE) of linear regression:

$$\frac{1}{n}\sum_{i=1}^{n}\mathbb{E}\{(Y_{i}^{\text{new}}-\hat{f}(X_{i}))^{2}\} = \frac{1}{n}\sum_{i=1}^{n}\{\mathbb{E}(\hat{\beta}^{\top}X_{i}-f(X_{i}))\}^{2}+\frac{K}{n}\sigma^{2}+\sigma^{2}$$

model complexity ⇒ penalty

## C<sub>p</sub> Statistic, Akaike and Bayesian Information Criteria

- How to estimate the sample average prediction error for a new data set (i.e., test data)?
- Use of training data ⇒ (typically) downward bias:

SAPE = 
$$\frac{1}{n} \sum_{i=1}^{n} L(Y_i^{\text{train}}, \hat{f}(X_i)) + \frac{1}{n} \sum_{i=1}^{n} \text{Cov}(\hat{Y}_i^{\text{test}}, Y_i^{\text{test}})$$

• Linear regression with squared error:

$$C_p = \frac{1}{n} \sum_{i=1}^{n} (\hat{\epsilon}_i^{\text{train}})^2 + \frac{2K}{n} \hat{\sigma}_{\text{train}}^2$$

• Maximum likelihood with deviance:

$$\frac{AIC}{n} = -2 \cdot \text{loglikelihood} + \frac{2K}{n} \xrightarrow{p} -2 \cdot \mathbb{E}(\text{loglikelihood}_i)$$

- Bayesian Information Criterion: BIC =  $-2 \cdot log likelihood + K \cdot log n$
- Select the model with the smallest  $C_D/AIC/BIC$

### **Cross Validation**

- Data are scarce ⇒ cannot create a separate validation set
- K-fold cross validation:



Estimated average population prediction error:

$$\mathbb{E}\{(Y_i^{\widehat{\mathsf{new}}} - \hat{f}(X_i))^2\} = \frac{1}{n} \sum_{i=1}^N L(Y_i, \hat{f}^{-\kappa(i)}(X_i))$$

where  $\hat{f}^{-\kappa(i)}(\cdot)$  is the fitted model without the group  $\kappa(i)$  to which observation i belongs

• leave-one-out cross validation (K = n): unbiased but high variance, also computationally demanding

## **Concluding Remarks**

- Likelihood inference: very general and powerful tool
- Asymptotic consistency and efficiency
- Report quantities of interest rather than model parameters
- Be aware of what "robust" standard error can and cannot do
- Parametric assumptions need to be made with care
- Model selection and validation: predictive criteria