### Econ 722 - Advanced Econometrics IV, Part II

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# Lecture #1 – AIC-type Information Criteria

Kullback-Leibler Divergence

Bias of Maximized Sample Log-Likelihood

Review of Asymptotics for Mis-specified MLE

Deriving AIC and TIC

Corrected AIC (AIC<sub>c</sub>)

# Kullback-Leibler (KL) Divergence

#### Motivation

How well does a given density f(y) approximate an unknown true density g(y)? Use this to select between parametric models.

#### Definition

$$\mathsf{KL}(g;f) = \underbrace{\mathbb{E}_G\left[\log\left\{\frac{g(Y)}{f(Y)}\right\}\right]}_{\mathsf{True\ density\ on\ top}} = \underbrace{\mathbb{E}_G\left[\log g(Y)\right]}_{\mathsf{Depends\ only\ on\ truth}} - \underbrace{\mathbb{E}_G\left[\log f(Y)\right]}_{\mathsf{Expected\ log-likelihood}}$$

#### **Properties**

- Not symmetric:  $KL(g; f) \neq KL(f; g)$
- ▶ By Jensen's Inequality:  $KL(g; f) \ge 0$  (strict iff g = f a.e.)

# KL Divergence and Mis-specified MLE

#### Pseudo-true Parameter Value $\theta_0$

$$\widehat{\theta}_{\mathit{MLE}} \overset{p}{\to} \theta_0 \equiv \operatorname*{arg\,min}_{\theta \in \Theta} \mathsf{KL}(g; f_\theta) = \operatorname*{arg\,max}_{\theta \in \Theta} \mathbb{E}_G[\log f(Y|\theta)]$$

What if  $f_{\theta}$  is correctly specified?

If  $g = f_{\theta}$  for some  $\theta$  then  $KL(g; f_{\theta})$  is minimized at zero.

Goal: Compare Mis-specified Models

$$\mathbb{E}_G [\log f(Y|\theta_0)]$$
 versus  $\mathbb{E}_G [\log h(Y|\gamma_0)]$ 

where  $\theta_0$  is the pseudo-true parameter value for  $f_\theta$  and  $\gamma_0$  is the pseudo-true parameter value for  $h_\gamma$ .

# How to Estimate Expected Log Likelihood?

For simplicity:  $Y_1, \ldots, Y_n \sim \text{ iid } g(y)$ 

#### Unbiased but Infeasible

$$\mathbb{E}_{G}\left[\frac{1}{T}\ell(\theta_{0})\right] = \mathbb{E}_{G}\left[\frac{1}{T}\sum_{t=1}^{T}\log f(Y_{t}|\theta_{0})\right] = \mathbb{E}_{G}\left[\log f(Y|\theta_{0})\right]$$

#### Biased but Feasible

 $T^{-1}\ell(\widehat{\theta}_{MLE})$  is a biased estimator of  $\mathbb{E}_G[\log f(Y|\theta_0)]$ .

#### Intuition for the Bias

 $T^{-1}\ell(\widehat{\theta}_{MLE}) > T^{-1}\ell(\theta_0)$  unless  $\widehat{\theta}_{MLE} = \theta_0$ . Maximized sample log-like. is an overly optimistic estimator of expected log-like.

### What to do about this bias?

- General-purpose asymptotic approximation of "degree of over-optimism" of maximized sample log-likelihood.
  - Takeuchi's Information Criterion (TIC)
  - Akaike's Information Criterion (AIC)
- 2. Problem-specific finite sample approach, assuming  $g \in f_{\theta}$ .
  - ► Corrected AIC (AIC<sub>c</sub>) of Hurvich and Tsai (1989)

#### **Tradeoffs**

TIC is most general and makes weakest assumptions, but requires very large T to work well. AIC is a good approximation to TIC that requires less data. Both AIC and TIC perform poorly when T is small relative to the number of parameters, hence AIC<sub>C</sub>.

# Recall: Asymptotics for Mis-specified ML Estimation

Model  $f(y|\theta)$ , pseudo-true parameter  $\theta_0$ . For simplicity  $Y_1, \ldots, Y_T \sim \text{ iid } g(y)$ .

#### Fundamental Expansion

$$\sqrt{T}(\widehat{\theta} - \theta_0) = J^{-1}\left(\sqrt{T}\,\overline{U}_T\right) + o_p(1)$$

$$J = -\mathbb{E}_G \left[ \frac{\partial \log f(Y|\theta_0)}{\partial \theta \partial \theta'} \right], \quad \bar{U}_T = \frac{1}{T} \sum_{t=1}^{I} \frac{\partial \log f(Y_t|\theta_0)}{\partial \theta}$$

#### Central Limit Theorem

$$\sqrt{T}\bar{U}_T \to_d U \sim N_p(0,K), \quad K = \operatorname{Var}_G \left[ \frac{\partial \log f(Y|\theta_0)}{\partial \theta} \right]$$

$$\sqrt{T}(\widehat{\theta}-\theta_0) 
ightarrow_d J^{-1}U \sim N_p(0,J^{-1}KJ^{-1})$$

#### Information Matrix Equality

If 
$$g = f_{\theta}$$
 for some  $\theta \in \Theta$  then  $K = J \implies \mathsf{AVAR}(\widehat{\theta}) = J^{-1}$ 

# Bias Relative to Infeasible Plug-in Estimator

#### Definition of Bias Term B

$$B = \underbrace{\frac{1}{T}\ell(\widehat{\theta})}_{\text{feasible overly-optimistic}} - \underbrace{\int g(y)\log f(y|\widehat{\theta}) \ dy}_{\text{uses data only once infeas. not overly-optimistic}}$$

#### Question to Answer

On average, over the sampling distribution of  $\widehat{\theta}$ , how large is B? AIC and TIC construct an asymptotic approximation of  $\mathbb{E}[B]$ .

# Derivation of AIC/TIC

### Step 1: Taylor Expansion

$$B = \bar{Z}_T + (\widehat{\theta} - \theta_0)'J(\widehat{\theta} - \theta_0) + o_p(T^{-1})$$

$$\bar{Z}_T = \frac{1}{T}\sum_{t=1}^T \{\log f(Y_t|\theta_0) - \mathbb{E}_G[\log f(Y|\theta_0)]\}$$

Step 2: 
$$\mathbb{E}[\bar{Z}_T] = 0$$

$$\mathbb{E}[B] \approx \mathbb{E}\left[ (\widehat{\theta} - \theta_0)' J(\widehat{\theta} - \theta_0) \right]$$

Step 3: 
$$\sqrt{T}(\widehat{\theta} - \theta_0) \rightarrow_d J^{-1}U$$

$$T(\widehat{\theta} - \theta_0)'J(\widehat{\theta} - \theta_0) \rightarrow_d U'J^{-1}U$$

# Derivation of AIC/TIC Continued...

Step 3: 
$$\sqrt{T}(\widehat{\theta} - \theta_0) \to_d J^{-1}U$$

$$T(\widehat{\theta} - \theta_0)'J(\widehat{\theta} - \theta_0) \to_d U'J^{-1}U$$

Step 4: 
$$U \sim N_p(0, K)$$
 
$$\mathbb{E}[B] \approx \frac{1}{T} \mathbb{E}[U'J^{-1}U] = \frac{1}{T} \text{tr} \left\{ J^{-1}K \right\}$$

#### Final Result:

 $T^{-1} {\rm tr} \left\{ J^{-1} K \right\}$  is an asymp. unbiased estimator of the over-optimism of  $T^{-1} \ell(\widehat{\theta})$  relative to  $\int g(y) \log f(y|\widehat{\theta}) \ dy$ .

#### TIC and AIC

#### Takeuchi's Information Criterion

Multiply by 
$$2T$$
, estimate  $J, K \Rightarrow \mathsf{TIC} = 2\left[\ell(\widehat{\theta}) - \mathsf{tr}\left\{\widehat{J}^{-1}\widehat{K}\right\}\right]$ 

#### Akaike's Information Criterion

If 
$$g = f_{ heta}$$
 then  $J = K \Rightarrow \operatorname{tr}\left\{J^{-1}K\right\} = p \Rightarrow \mathsf{AIC} = 2\left[\ell(\widehat{ heta}) - p\right]$ 

### Contrasting AIC and TIC

Technically, AIC requires that all models under consideration are at least correctly specified while TIC doesn't. But  $J^{-1}K$  is hard to estimate, and if a model is badly mis-specified,  $\ell(\widehat{\theta})$  dominates.

# Corrected AIC (AIC<sub>c</sub>) – Hurvich & Tsai (1989)

#### Idea Behind AIC

Asymptotic approximation used for AIC/TIC works poorly if p is too large relative to T. Try exact, finite-sample approach instead.

Assumption: True DGP

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta}_0 + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim \mathit{N}(\mathbf{0}, \sigma_0^2 \mathbf{I}_T), \quad \textit{k} \; \mathsf{Regressors}$$

Can Show That

$$\mathit{KL}(g,f) = rac{T}{2} \left[ rac{\sigma_0^2}{\sigma_1^2} - \log \left( rac{\sigma_0^2}{\sigma_1^2} 
ight) - 1 
ight] + \left( rac{1}{2\sigma_1^2} 
ight) (eta_0 - eta_1)' \mathbf{X}' \mathbf{X} (eta_0 - eta_1)$$

Where f is a normal regression model with parameters  $(\beta_1, \sigma_1^2)$  that might not be the true parameters.

### But how can we use this?

$$\mathit{KL}(g,f) = rac{T}{2} \left[ rac{\sigma_0^2}{\sigma_1^2} - \log \left( rac{\sigma_0^2}{\sigma_1^2} 
ight) - 1 
ight] + \left( rac{1}{2\sigma_1^2} 
ight) (eta_0 - eta_1)' \mathbf{X}' \mathbf{X} (eta_0 - eta_1)$$

- 1. Would need to know  $(\beta_1, \sigma_1^2)$  for candidate model.
  - Easy: just use MLE  $(\widehat{\boldsymbol{\beta}}_1, \widehat{\sigma}_1^2)$
- 2. Would need to know  $(\beta_0, \sigma_0^2)$  for true model.
  - Very hard! The whole problem is that we don't know these!

### Hurvich & Tsai (1989) Assume:

- Every candidate model is at least correctly specified
- ▶ Implies any candidate estimator  $(\widehat{\beta}, \widehat{\sigma}^2)$  is consistent for truth.

# Deriving the Corrected AIC

Since  $(\widehat{\beta}, \widehat{\sigma}^2)$  are random, look at  $\mathbb{E}[\widehat{KL}]$ , where

$$\widehat{\mathit{KL}} = \frac{\mathit{T}}{2} \left[ \frac{\sigma_0^2}{\widehat{\sigma}^2} - \log \left( \frac{\sigma_0^2}{\widehat{\sigma}^2} \right) - 1 \right] + \left( \frac{1}{2\widehat{\sigma}^2} \right) (\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)' \mathbf{X}' \mathbf{X} (\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)$$

Finite-sample theory for correctly spec. normal regression model:

$$\mathbb{E}\left[\widehat{\mathit{KL}}\right] = \frac{T}{2} \left\{ \frac{T+k}{T-k-2} - \log(\sigma_0^2) + \mathbb{E}[\log \widehat{\sigma}^2] - 1 \right\}$$

Eliminate constants and scaling, unbiased estimator of  $\mathbb{E}[\log \widehat{\sigma}^2]$ :

$$AIC_c = \log \widehat{\sigma}^2 + \frac{T+k}{T-k-2}$$

a finite-sample unbiased estimator of KL for model comparison

### Lecture #2 – More on "Classical" Model Selection

Mallow's  $C_p$ 

Bayesian Model Comparison

Laplace Approximation

Bayesian Information Criterion (BIC)

# Motivation: Predict **y** from **x** via Linear Regression

$$egin{aligned} \mathbf{y} &= \mathbf{X} & \boldsymbol{\beta} \\ ( au imes \mathbf{1}) &= ( au imes K)(K imes \mathbf{1}) \end{aligned} + oldsymbol{\epsilon} \ \mathbb{E}[oldsymbol{\epsilon}|\mathbf{X}] = 0, \quad \mathsf{Var}(oldsymbol{\epsilon}|\mathbf{X}) = \sigma^2 \mathbf{I} \end{aligned}$$

- If β were known, could never achieve lower MSE than by using all regressors to predict.
- ▶ But \(\beta\) is unknown so we have to estimate it from data \(\Rightarrow\) bias-variance tradeoff.
- Could make sense to exclude regressors with small coefficients: add small bias but reduce variance.

# Operationalizing the Bias-Variance Tradeoff Idea

### Mallow's $C_p$

Approximate the predictive MSE of each model relative to the infeasible optimum in which  $oldsymbol{eta}$  is known.

#### Notation

- ▶ Model index m and regressor matrix  $X_m$
- ▶ Corresponding OLS estimator  $\widehat{\beta}_m$  padded out with zeros
- $\mathbf{X}\widehat{\boldsymbol{\beta}}_m = \mathbf{X}_{(-m)}\mathbf{0} + \mathbf{X}_m \left[ (\mathbf{X}_m'\mathbf{X}_m)^{-1}\mathbf{X}_m'\mathbf{y} \right] = \mathbf{P}_m\mathbf{y}$

# In-sample versus Out-of-sample Prediction Error

### Why not compare RSS(m)?

In-sample prediction error:  $RSS(m) = (\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}_m)'(\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}_m)$ 

#### From your Problem Set

RSS cannot decrease even if we add irrelevant regressors. Thus in-sample prediction error is an overly optimistic estimate of out-of-sample prediction error.

#### Bias-Variance Tradeoff

Out-of-sample performance of full model (using all regressors) could be very poor if there is a lot of estimation uncertainty associated with regressors that aren't very predictive.

# Predictive MSE of $\mathbf{X}\widehat{\boldsymbol{\beta}}_m$ relative to infeasible optimum $\mathbf{X}\boldsymbol{\beta}$

Step 1: Algebra

$$\mathbf{X}\widehat{\boldsymbol{\beta}}_{m} - \mathbf{X}\boldsymbol{\beta} = \mathbf{P}_{m}\mathbf{y} - \mathbf{X}\boldsymbol{\beta} = \mathbf{P}_{m}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) - (\mathbf{I} - \mathbf{P}_{m})\mathbf{X}\boldsymbol{\beta}$$

$$= \mathbf{P}_{m}\boldsymbol{\epsilon} - (\mathbf{I} - \mathbf{P}_{m})\mathbf{X}\boldsymbol{\beta}$$

Step 2:  $P_m$  and  $(I - P_m)$  are symmetric, idempotent, and orthogonal

$$\begin{aligned} \left| \left| \mathbf{X} \widehat{\boldsymbol{\beta}}_{m} - \mathbf{X} \boldsymbol{\beta} \right| \right|^{2} &= \left\{ \mathbf{P}_{m} \boldsymbol{\epsilon} - (\mathbf{I} - \mathbf{P}_{m}) \mathbf{X} \boldsymbol{\beta} \right\}' \left\{ \mathbf{P}_{m} \boldsymbol{\epsilon} + (\mathbf{I} - \mathbf{P}_{m}) \mathbf{X} \boldsymbol{\beta} \right\} \\ &= \left. \boldsymbol{\epsilon}' \mathbf{P}'_{m} \mathbf{P}_{m} \boldsymbol{\epsilon} - \boldsymbol{\beta}' \mathbf{X}' (\mathbf{I} - \mathbf{P}_{m})' \mathbf{P}_{m} \boldsymbol{\epsilon} - \boldsymbol{\epsilon}' \mathbf{P}'_{m} (\mathbf{I} - \mathbf{P}_{m}) \mathbf{X} \boldsymbol{\beta} \right. \\ &+ \left. \boldsymbol{\beta}' \mathbf{X}' (\mathbf{I} - \mathbf{P}_{m}) (\mathbf{I} - \mathbf{P}_{m}) \mathbf{X} \boldsymbol{\beta} \right. \\ &= \left. \boldsymbol{\epsilon}' \mathbf{P}_{m} \boldsymbol{\epsilon} + \boldsymbol{\beta}' \mathbf{X}' (\mathbf{I} - \mathbf{P}_{m}) \mathbf{X} \boldsymbol{\beta} \end{aligned}$$

# Predictive MSE of $\mathbf{X}\hat{\boldsymbol{\beta}}_m$ relative to infeasible optimum $\mathbf{X}\boldsymbol{\beta}$

### Step 3: Expectation of Step 2 conditional on X

$$\begin{aligned} \mathsf{MSE}(m|\mathbf{X}) &= & \mathbb{E}\left[(\mathbf{X}\widehat{\boldsymbol{\beta}}_m - \mathbf{X}\boldsymbol{\beta})'(\mathbf{X}\widehat{\boldsymbol{\beta}}_m - \mathbf{X}\boldsymbol{\beta})|\mathbf{X}\right] \\ &= & \mathbb{E}\left[\epsilon'\mathbf{P}_m\boldsymbol{\epsilon}|\mathbf{X}\right] + \mathbb{E}\left[\boldsymbol{\beta}'\mathbf{X}'(\mathbf{I} - \mathbf{P}_m)\mathbf{X}\boldsymbol{\beta}|\mathbf{X}\right] \\ &= & \mathbb{E}\left[\mathsf{tr}\left\{\epsilon'\mathbf{P}_m\boldsymbol{\epsilon}\right\}|\mathbf{X}\right] + \boldsymbol{\beta}'\mathbf{X}'(\mathbf{I} - \mathbf{P}_m)\mathbf{X}\boldsymbol{\beta} \\ &= & \mathsf{tr}\left\{\mathbb{E}[\boldsymbol{\epsilon}\boldsymbol{\epsilon}'|\mathbf{X}]\mathbf{P}_m\right\} + \boldsymbol{\beta}'\mathbf{X}'(\mathbf{I} - \mathbf{P}_m)\mathbf{X}\boldsymbol{\beta} \\ &= & \mathsf{tr}\left\{\sigma^2\mathbf{P}_m\right\} + \boldsymbol{\beta}'\mathbf{X}'(\mathbf{I} - \mathbf{P}_m)\mathbf{X}\boldsymbol{\beta} \\ &= & \sigma^2k_m + \boldsymbol{\beta}'\mathbf{X}'(\mathbf{I} - \mathbf{P}_m)\mathbf{X}\boldsymbol{\beta} \end{aligned}$$

where  $k_m$  denotes the number of regressors in  $\mathbf{X}_m$  and  $\operatorname{tr}(\mathbf{P}_m) = \operatorname{tr}\left\{\mathbf{X}_m \left(\mathbf{X}_m'\mathbf{X}_m\right)^{-1}\mathbf{X}_m'\right\} = \operatorname{tr}\left\{\mathbf{X}_m'\mathbf{X}_m \left(\mathbf{X}_m'\mathbf{X}_m\right)^{-1}\right\} = \operatorname{tr}(\mathbf{I}_m)$ 

# Now we know the MSE of a given model...

$$MSE(m|\mathbf{X}) = \sigma^2 k_m + \beta' \mathbf{X}' (\mathbf{I} - \mathbf{P}_m) \mathbf{X} \beta$$

#### Bias-Variance Tradeoff

- ▶ Smaller Model  $\Rightarrow \sigma^2 k_m$  smaller: less estimation uncertainty.
- ▶ Bigger Model  $\Rightarrow \mathbf{X}'(\mathbf{I} \mathbf{P}_m)\mathbf{X} = ||(\mathbf{I} \mathbf{P}_m)\mathbf{X}||^2$  is in general smaller: less (squared) bias.

### Mallow's $C_p$

- ▶ Problem: MSE formula is infeasible since it involves  $\beta$  and  $\sigma^2$ .
- ▶ Solution: Mallow's  $C_p$  constructs an unbiased estimator.
- ▶ Idea: what about plugging in  $\widehat{\beta}$  to estimate second term?

# What if we plug in $\hat{\beta}$ to estimate the second term?

For the missing algebra in Step 4, see the lecture notes.

#### Notation

Let  $\widehat{\boldsymbol{\beta}}$  denote the full model estimator and  ${\bf P}$  be the corresponding projection matrix:  ${\bf X}\widehat{\boldsymbol{\beta}}={\bf P}{\bf y}.$ 

#### Crucial Fact

 $span(\mathbf{X}_m)$  is a subspace of  $span(\mathbf{X})$ , so  $\mathbf{P}_m\mathbf{P} = \mathbf{P}\mathbf{P}_m = \mathbf{P}_m$ .

Step 4: Algebra using the preceding fact

$$\mathbb{E}\left[\widehat{\boldsymbol{\beta}}'\mathbf{X}'(\mathbf{I}-\mathbf{P}_m)\mathbf{X}\widehat{\boldsymbol{\beta}}|\mathbf{X}\right]=\cdots=\boldsymbol{\beta}'\mathbf{X}'(\mathbf{I}-\mathbf{P}_m)\mathbf{X}\boldsymbol{\beta}+\mathbb{E}\left[\boldsymbol{\epsilon}'(\mathbf{P}-\mathbf{P}_m)\boldsymbol{\epsilon}|\mathbf{X}\right]$$

# Substituting $\widehat{\boldsymbol{\beta}}$ doesn't work...

Step 5: Use "Trace Trick" on second term from Step 4

$$\begin{split} \mathbb{E}[\epsilon'(\mathbf{P} - \mathbf{P}_m)\epsilon|\mathbf{X}] &= \mathbb{E}[\operatorname{tr}\left\{\epsilon'(\mathbf{P} - \mathbf{P}_m)\epsilon\right\}|\mathbf{X}] \\ &= \operatorname{tr}\left\{\mathbb{E}[\epsilon\epsilon'|\mathbf{X}](\mathbf{P} - \mathbf{P}_m)\right\} \\ &= \operatorname{tr}\left\{\sigma^2(\mathbf{P} - \mathbf{P}_m)\right\} \\ &= \sigma^2\left(\operatorname{trace}\left\{\mathbf{P}\right\} - \operatorname{trace}\left\{\mathbf{P}_m\right\}\right) \\ &= \sigma^2(K - k_m) \end{split}$$

where K is the total number of regressors in X

Bias of Plug-in Estimator

$$\mathbb{E}\left[\widehat{\boldsymbol{\beta}}'\mathbf{X}'(\mathbf{I}-\mathbf{P}_m)\mathbf{X}\widehat{\boldsymbol{\beta}}|\mathbf{X}\right] = \underbrace{\boldsymbol{\beta}'\mathbf{X}'(\mathbf{I}-\mathbf{P}_m)\mathbf{X}\boldsymbol{\beta}}_{\text{Truth}} + \underbrace{\boldsymbol{\sigma}^2(\boldsymbol{K}-\boldsymbol{k}_m)}_{\text{Bias}}$$

# Putting Everything Together: Mallow's $C_p$

Want An Unbiased Estimator of This:

$$\mathsf{MSE}(m|\mathbf{X}) = \sigma^2 k_m + \beta' \mathbf{X}' (\mathbf{I} - \mathbf{P}_m) \mathbf{X} \boldsymbol{\beta}$$

#### Previous Slide:

$$\mathbb{E}\left[\widehat{\boldsymbol{\beta}}'\mathbf{X}'(\mathbf{I}-\mathbf{P}_m)\mathbf{X}\widehat{\boldsymbol{\beta}}|\mathbf{X}\right] = \boldsymbol{\beta}'\mathbf{X}'(\mathbf{I}-\mathbf{P}_m)\mathbf{X}\boldsymbol{\beta} + \sigma^2(K-k_m)$$

#### End Result:

$$MC(m) = \widehat{\sigma}^2 k_m + \left[ \widehat{\beta}' \mathbf{X}' (\mathbf{I} - \mathbf{P}_m) \mathbf{X} \widehat{\beta} - \widehat{\sigma}^2 (K - k_m) \right]$$
$$= \widehat{\beta}' \mathbf{X}' (\mathbf{I} - \mathbf{P}_m) \mathbf{X} \widehat{\beta} + \widehat{\sigma}^2 (2k_m - K)$$

is an unbiased estimator of MSE, with  $\hat{\sigma}^2 = \mathbf{y}'(\mathbf{I} - \mathbf{P})\mathbf{y}/(T - K)$ 

# Why is this different from the textbook formula?

Just algebra, but tedious...

$$\begin{aligned} \mathsf{MC}(m) - 2\widehat{\sigma}^2 k_m &= \widehat{\beta}' X' (\mathbf{I} - P_M) X \widehat{\beta} - K \widehat{\sigma}^2 \\ \vdots &&\\ &= \mathbf{y}' (\mathbf{I} - P_M) \mathbf{y} - T \widehat{\sigma}^2 \\ &= \mathsf{RSS}(m) - T \widehat{\sigma}^2 \end{aligned}$$

Therefore:

$$MC(m) = RSS(m) + \widehat{\sigma}^2(2k_m - T)$$

Divide Through by  $\widehat{\sigma}^2$ :

$$C_p(m) = \frac{\mathsf{RSS}(m)}{\widehat{\sigma}^2} + 2k_m - T$$

Tells us how to adjust RSS for number of regressors...

# Bayesian Model Comparison: Marginal Likelihoods

### Bayes' Rule for Model $m \in \mathcal{M}$

$$\underbrace{\frac{\pi(\boldsymbol{\theta}|\mathbf{y},m)}_{\mathsf{Posterior}} \propto \underbrace{\pi(\boldsymbol{\theta}|m)}_{\mathsf{Prior}} \underbrace{f(\mathbf{y}|\boldsymbol{\theta},m)}_{\mathsf{Likelihood}}}_{\mathsf{Likelihood}}$$

$$\underbrace{f(\mathbf{y}|m)}_{\mathsf{Marginal Likelihood}} = \int_{\Theta} \pi(\boldsymbol{\theta}|m) f(\mathbf{y}|\boldsymbol{\theta},m) \; \mathrm{d}\boldsymbol{\theta}$$

### Posterior Model Probability for $m \in \mathcal{M}$

$$P(m|\mathbf{y}) = \frac{P(m)f(\mathbf{y}|m)}{f(\mathbf{y})} = \frac{\int_{\Theta} P(m)f(\mathbf{y}, \boldsymbol{\theta}|m) d\boldsymbol{\theta}}{f(\mathbf{y})} = \frac{P(m)}{f(\mathbf{y})} \int_{\Theta} \pi(\boldsymbol{\theta}|m)f(\mathbf{y}|\boldsymbol{\theta}, m) d\boldsymbol{\theta}$$

where P(m) is the prior model probability and f(y) is constant across models.

# Laplace (aka Saddlepoint) Approximation

Suppress model index m for simplicity.

General Case: for T large...

$$\int_{\Theta} g(\boldsymbol{\theta}) \exp\{T \cdot h(\boldsymbol{\theta})\} \; \mathrm{d}\boldsymbol{\theta} \approx \left(\frac{2\pi}{T}\right)^{p/2} \exp\{T \cdot h(\boldsymbol{\theta}_0)\} g(\boldsymbol{\theta}_0) \left|H(\boldsymbol{\theta}_0)\right|^{-1/2}$$

$$p = \dim(\theta), \ \theta_0 = \arg\max_{\theta \in \Theta} h(\theta), \ H(\theta_0) = -\frac{\partial^2 h(\theta)}{\partial \theta \partial \theta'} \Big|_{\theta = \theta_0}$$

### Use to Approximate Marginal Likelihood

$$h(\theta) = \frac{\ell(\theta)}{T} = \frac{1}{T} \sum_{t=1}^{T} \log f(Y_i | \theta), \quad H(\theta) = J_T(\theta) = -\frac{1}{T} \sum_{t=1}^{T} \frac{\partial^2 \log f(Y_i | \theta)}{\partial \theta \partial \theta'}, \quad g(\theta) = \pi(\theta)$$

and substitute  $\widehat{\boldsymbol{\theta}}_{MF}$  for  $\boldsymbol{\theta}_0$ 

# Laplace Approximation to Marginal Likelihood

Suppress model index m for simplicity.

$$\int_{\Theta} \pi(\boldsymbol{\theta}) f(\mathbf{y}|\boldsymbol{\theta}) d\boldsymbol{\theta} \approx \left(\frac{2\pi}{T}\right)^{p/2} \exp\left\{\ell(\widehat{\boldsymbol{\theta}}_{MLE})\right\} \pi(\widehat{\boldsymbol{\theta}}_{MLE}) \left|J_{T}(\widehat{\boldsymbol{\theta}}_{MLE})\right|^{-1/2}$$

$$\ell(\boldsymbol{\theta}) = \sum_{i=1}^{T} \log f(Y_{i}|\boldsymbol{\theta}), \quad H(\boldsymbol{\theta}) = J_{T}(\boldsymbol{\theta}) = -\frac{1}{T} \sum_{i=1}^{T} \frac{\partial^{2} \log f(Y_{i}|\boldsymbol{\theta})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}'}$$

# Bayesian Information Criterion

$$\int_{\Theta} \pi(\boldsymbol{\theta}) f(\mathbf{y}|\boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{\theta} \approx \left(\frac{2\pi}{T}\right)^{p/2} \exp\left\{\ell(\widehat{\boldsymbol{\theta}}_{\mathit{MLE}})\right\} \pi(\widehat{\boldsymbol{\theta}}_{\mathit{MLE}}) \left|J_{T}(\widehat{\boldsymbol{\theta}}_{\mathit{MLE}})\right|^{-1/2}$$

Take Logs and Multiply by 2

$$2\log f(\mathbf{y}|\boldsymbol{\theta}) \approx \underbrace{2\ell(\widehat{\boldsymbol{\theta}}_{MLE})}_{O_p(T)} - \underbrace{p\log(T)}_{O(\log T)} + \underbrace{p\log(2\pi) + \log \pi(\widehat{\boldsymbol{\theta}}) - \log|J_T(\widehat{\boldsymbol{\theta}})|}_{O_p(1)}$$

#### The BIC

Assume uniform prior over models and ignore lower order terms:

$$BIC(m) = 2 \log f(\mathbf{y}|\widehat{\boldsymbol{\theta}}, m) - p_m \log(T)$$

large-sample Frequentist approx. to Bayesian marginal likelihood

### Lecture #3 – Cross-Validation

Model selection via a Hold-out Sample

K-fold Cross-validation

Asymptotic Equivalence Between LOO-CV and TIC

Influence Functions

# Model Selection using a Hold-out Sample

- The real problem is double use of the data: first for estimation, then for model comparison.
  - Maximized sample log-likelihood is an overly optimistic estimate of expected log-likelihood and hence KL-divergence
  - ► In-sample squared prediction error is an overly optimistic estimator of out-of-sample squared prediction error
- ► AIC/TIC, AIC<sub>c</sub>, BIC, C<sub>p</sub> penalize sample log-likelihood or RSS to compensate.

Another idea: don't re-use the same data!

### Hold-out Sample: Partition the Full Dataset



Unfortunately this is extremely wasteful of data...

# K-fold Cross-Validation: "Pseudo-out-of-sample"



### Step 1

Randomly partition full dataset into K folds of approx. equal size.

### Step 2

Treat  $k^{\text{th}}$  fold as a hold-out sample and estimate model using all observations except those in fold k: yielding estimator  $\widehat{\theta}(-k)$ .

# K-fold Cross-Validation: "Pseudo-out-of-sample"

### Step 2

Treat  $k^{\text{th}}$  fold as a hold-out sample and estimate model using all observations except those in fold k: yielding estimator  $\widehat{\theta}(-k)$ .

### Step 3

Repeat Step 2 for each k = 1, ..., K.

### Step 4

For each t calculate the prediction  $\hat{y}_t^{-k(t)}$  of  $y_t$  based on  $\hat{\theta}(-k(t))$ , the estimator that excluded observation t.

# K-fold Cross-Validation: "Pseudo-out-of-sample"

### Step 4

For each t calculate the prediction  $\hat{y}_t^{-k(t)}$  of  $y_t$  based on  $\hat{\theta}(-k(t))$ , the estimator that excluded observation t.

### Step 5

Define  $CV_K = \frac{1}{T} \sum_{t=1}^{T} L\left(y_t, \widehat{y}_t^{-k(t)}\right)$  where L is a loss function.

### Step 5

Repeat for each model & choose m to minimize  $CV_K(m)$ .

CV uses each observation for parameter estimation and model evaluation but never at the same time!

# Cross-Validation (CV): Some Details

#### Which Loss Function?

- For regression squared error loss makes sense
- For classification (discrete prediction) could use zero-one loss.
- ► Can also use log-likelihood/KL-divergence as a loss function. . .

### How Many Folds?

- ▶ One extreme: K = 2. Closest to Training/Test idea.
- ▶ Other extreme: K = T Leave-one-out CV (LOO-CV).
- Computationally expensive model ⇒ may prefer fewer folds.
- ▶ If your model is a linear smoother there's a computational trick that makes LOO-CV extremely fast. (Problem Set)
- Asymptotic properties are related to K...

## Relationship between LOO-CV and TIC

#### **Theorem**

LOO-CV using KL-divergence as the loss function is asymptotically equivalent to TIC but doesn't require us to estimate the Hessian and variance of the score.

### Large-sample Equivalence of LOO-CV and TIC

#### Notation and Assumptions

For simplicity let  $Y_1,\ldots,Y_T\sim \mathrm{iid}$ . Let  $\widehat{\theta}_{(t)}$  be the maximum likelihood estimator based on all observations except t and  $\widehat{\theta}$  be the full-sample estimator.

### Log-likelihood as "Loss"

 $\mathsf{CV}_1 = \frac{1}{T} \sum_{t=1}^T \log f(y_t | \widehat{\theta}_{(t)})$  but since min.  $\mathsf{KL} = \mathsf{max}$ . log-like. we choose the model with highest  $\mathsf{CV}_1(m)$ .

### Overview of the Proof

First-Order Taylor Expansion of  $\widehat{\theta}_{(t)}$  around  $\widehat{\theta}$ :

$$CV_{1} = \frac{1}{T} \sum_{t=1}^{T} \log f(y_{t}|\widehat{\theta}_{(t)})$$

$$= \frac{1}{T} \sum_{t=1}^{T} \left[ \log f(y_{t}|\widehat{\theta}) + \frac{\partial \log f(y_{t}|\widehat{\theta})}{\partial \theta'} \left( \widehat{\theta}_{(t)} - \widehat{\theta} \right) \right] + o_{p}(1)$$

$$= \frac{\ell(\widehat{\theta})}{T} + \frac{1}{T} \sum_{t=1}^{T} \frac{\partial \log f(y_{t}|\widehat{\theta})}{\partial \theta'} \left( \widehat{\theta}_{(t)} - \widehat{\theta} \right) + o_{p}(1)$$

Crucial point: the first-order term is not zero in this case. (Why?)

### Overview of Proof

From expansion on previous slide, we simply need to show that:

$$\frac{1}{T} \sum_{t=1}^{T} \frac{\partial \log f(y_t | \widehat{\theta})}{\partial \theta'} \left( \widehat{\theta}_{(t)} - \widehat{\theta} \right) = -\frac{1}{T} \operatorname{tr} \left( \widehat{J}^{-1} \widehat{K} \right) + o_p(1)$$

$$\widehat{K} = \frac{1}{T} \sum_{t=1}^{T} \left( \frac{\partial \log f(y_t | \widehat{\theta})}{\partial \theta} \right) \left( \frac{\partial \log f(y_t | \widehat{\theta})}{\partial \theta} \right)'$$

$$\widehat{J} = -\frac{1}{T} \sum_{t=1}^{T} \frac{\partial \log f(y_t | \widehat{\theta})}{\partial \theta \partial \theta'}$$

### Overview of Proof

By the definition of  $\widehat{K}$  and the properties of the trace operator:

$$\begin{split} -\frac{1}{T} \mathrm{tr} \left\{ \widehat{J}^{-1} \widehat{K} \right\} &= -\frac{1}{T} \mathrm{tr} \left\{ \widehat{J}^{-1} \left[ \frac{1}{T} \sum_{t=1}^{T} \left( \frac{\partial \log f(y_t | \widehat{\theta})}{\partial \theta} \right) \left( \frac{\partial \log f(y_t | \widehat{\theta})}{\partial \theta} \right)' \right] \right\} \\ &= \left[ \frac{1}{T} \sum_{t=1}^{T} \mathrm{tr} \left\{ \frac{-\widehat{J}^{-1}}{T} \left( \frac{\partial \log f(y_t | \widehat{\theta})}{\partial \theta} \right) \left( \frac{\partial \log f(y_t | \widehat{\theta})}{\partial \theta} \right)' \right\} \right] \\ &= \frac{1}{T} \sum_{t=1}^{T} \frac{\partial \log f(y_t | \widehat{\theta})}{\partial \theta'} \left( -\frac{1}{T} \widehat{J}^{-1} \right) \frac{\partial \log f(y_t | \widehat{\theta})}{\partial \theta} \end{split}$$

So it suffices to show that

$$\left(\widehat{ heta}_{(t)} - \widehat{ heta}
ight) = -rac{1}{T}\widehat{J}^{-1}\left[rac{\partial \log f(y_t|\widehat{ heta})}{\partial heta}
ight] + o_p(1)$$

## Digression: Functionals and Influence Functions

### (Statistical) Functional

 $\mathbb{T} = \mathbb{T}(G)$  maps a CDF G to  $\mathbb{R}^p$ .

### Example: ML Estimation

$$heta_0 = \mathbb{T}(G) = \operatorname*{arg\,min}_{\theta \in \Theta} E_G \left[ \log \left\{ rac{g(Y)}{f(Y|\theta)} 
ight\} 
ight]$$

#### Influence Function

Let  $\delta_y$  be a point mass at y:  $\delta_y(y) = 1$ ,  $\delta_y(y') = 0$  for  $y' \neq y$ . Influence function = functional derivative: how does a small change in G affect  $\mathbb{T}$ ?

$$\inf(G, y) = \lim_{\epsilon \to 0} \frac{\mathbb{T}\left[(1 - \epsilon) G + \epsilon \delta_y\right] - \mathbb{T}(G)}{\epsilon}$$

### Back to the Proof...

#### Step 1

The influence function for ML estimation turns out to be  $\inf(G, y) = J^{-1} \frac{\partial}{\partial \theta} \log f(y|\theta_0).$ 

#### Step 2

Let  $\widehat{G}$  denote the empirical CDF based on  $y_1, \ldots, y_T$ . Then:

$$\left(\widehat{\theta}_{(t)} - \widehat{\theta}\right) = -\frac{1}{T} \mathsf{infl}(\widehat{G}, y_t) + o_p(1)$$

### Step 3

Evaluating Step 1 at  $\widehat{G}$  and substituting into Step 2

$$\left(\widehat{ heta}_{(t)} - \widehat{ heta}
ight) = -rac{1}{T}\widehat{J}^{-1}\left[rac{\partial \log f(y_t|\widehat{ heta})}{\partial heta}
ight] + o_p(1)$$

### Lecture #4 – Asymptotic Properties

Overview

Weak Consistency

Consistency

AIC versus BIC in a Simple Example

### Overview

- ▶ What happens as  $T \to \infty$ ?
- Consistency: choose "best" model wpa 1
- Efficiency: procedure with good risk properties
- Can't have both at once.
- Large, fairly technical literature: only a brief overview today.
- More details: Sin and White (1992, 1996), Pötscher (1991),
   Leeb & Pötscher (2005), Yang (2005) and Yang (2007).

### Penalizing the Likelihood

### Examples we've seen:

$$\begin{split} & \textit{TIC} &= 2\ell_{\textit{T}}(\widehat{\theta}) - \mathsf{trace}\left\{\widehat{J}^{-1}\widehat{K}\right\} \\ & \textit{AIC} &= 2\ell_{\textit{T}}(\widehat{\theta}) - 2\,\mathsf{length}(\theta) \\ & \textit{BIC} &= 2\ell_{\textit{T}}(\widehat{\theta}) - \mathsf{log}(\textit{T})\,\mathsf{length}(\theta) \end{split}$$

Generic penalty  $c_{T,k}$ 

$$IC(M_k) = 2\sum_{t=1}^{T} \log f_{k,t}(Y_t|\widehat{\theta_k}) - c_{T,k}$$

How does choice of  $c_{T,k}$  affect behavior of the criterion?

## Weak Consistency: Suppose $M_{k_0}$ Uniquely Minimizes KL

### Assumption

$$\liminf_{T \to \infty} \left( \min_{k \neq k_0} \frac{1}{T} \sum_{t=1}^{T} \left\{ \mathit{KL}(g; f_{k,t}) - \mathit{KL}(g; f_{k_0,t}) \right\} \right) > 0$$

### Consequences

- Any criterion with c<sub>T,k</sub> > 0 and c<sub>T,k</sub> = o<sub>p</sub>(T) is weakly consistent: selects M<sub>k0</sub> wpa 1 in the limit.
- ▶ Weak consistency still holds if  $c_{T,k}$  is zero for one of the models, so long as it is strictly positive for all the others.

## Both AIC and BIC are Weakly Consistent

AIC and BIC are Weakly Consistent: both satisfy  $T^{-1}c_{T,k} \stackrel{p}{\to} 0$ .

BIC Penalty: 
$$c_{T,k} = \log(T) \times \operatorname{length}(\theta_k)$$

AIC Penalty: 
$$c_{T,k} = 2 \times \text{length}(\theta_k)$$

# Consistency

# Efficiency

## Consistency versus Efficiency in a Simple Example

#### Information Criteria

Consider criteria of the form  $IC_m = 2\ell(\theta) - d_T \times length(\theta)$ .

#### True DGP

$$Y_1, \ldots, Y_T \sim \text{iid N}(\mu, 1)$$

#### Candidate Models

 $M_0$  assumes  $\mu = 0$ ,  $M_1$  does not restrict  $\mu$ . Only one parameter:

$$egin{aligned} \mathsf{IC}_0 &= 2 \max_{\mu} \left\{ \ell(\mu) \colon \mathsf{M}_0 
ight\} \ &\mathsf{IC}_1 &= 2 \max_{\mu} \left\{ \ell(\mu) \colon \mathsf{M}_1 
ight\} - d_{\mathcal{T}} \end{aligned}$$

## Log-Likelihood Function

Since 
$$\sum_{t=1}^{T} (Y_t - \mu)^2 = T(\bar{Y} - \mu)^2 + T\hat{\sigma}^2$$
,

$$\begin{split} \ell_T(\mu) &= \sum_{t=1}^T \log \left( \frac{1}{2\pi} \exp \left\{ -\frac{1}{2} (Y_t - \mu)^2 \right\} \right) \\ &= -\frac{T}{2} \log (2\pi) - \frac{1}{2} \sum_{t=1}^T (Y_t - \mu)^2 \\ &= -\frac{T}{2} \log (2\pi) - \frac{T}{2} \widehat{\sigma}^2 - \frac{T}{2} (\bar{Y} - \mu)^2 \\ &= \operatorname{Constant} - \frac{T}{2} (\bar{Y} - \mu)^2 \end{split}$$

# Side Calculation: $\sum_{t=1}^{T} (Y_t - \mu)^2 = T(\bar{Y} - \mu)^2 + T\hat{\sigma}^2$

$$T\hat{\sigma}^{2} = \sum_{t=1}^{T} (Y_{t} - \bar{Y})^{2} = \sum_{t=1}^{T} (Y_{t} - \mu + \mu - \bar{Y})^{2} = \sum_{t=1}^{T} [(Y_{t} - \mu) - (\bar{Y} - \mu)]^{2}$$

$$= \sum_{t=1}^{T} (Y_{t} - \mu)^{2} - \sum_{t=1}^{T} 2(Y_{t} - \mu)(\bar{Y} - \mu) + \sum_{t=1}^{T} (\bar{Y} - \mu)^{2}$$

$$= \left[ \sum_{t=1}^{T} (Y_{t} - \mu)^{2} \right] - 2(\bar{Y} - \mu) \left( \sum_{t=1}^{T} Y_{t} - \sum_{t=1}^{T} \mu \right) + T(\bar{Y} - \mu)^{2}$$

$$= \left[ \sum_{t=1}^{T} (Y_{t} - \mu)^{2} \right] - 2(\bar{Y} - \mu)(T\bar{Y} - T\mu) + T(\bar{Y} - \mu)^{2}$$

$$= \left[ \sum_{t=1}^{T} (Y_{t} - \mu)^{2} \right] - 2T(\bar{Y} - \mu)^{2} + T(\bar{Y} - \mu)^{2}$$

$$= \left[ \sum_{t=1}^{T} (Y_{t} - \mu)^{2} \right] - T(\bar{Y} - \mu)^{2}$$

## The Selected Model $\widehat{M}$

#### Information Criteria

 $M_0$  sets  $\mu=0$  while  $M_1$  uses the MLE  $\bar{Y}$ , so we have

$$\mathsf{IC}_0 = 2\max_{\mu} \left\{ \ell(\mu) \colon \mathsf{M}_0 \right\} = 2 imes \mathsf{Constant} - \mathcal{T} ar{Y}^2$$
  $\mathsf{IC}_1 = 2\max_{\mu} \left\{ \ell(\mu) \colon \mathsf{M}_1 \right\} = 2 imes \mathsf{Constant} - d_{\mathcal{T}}$ 

#### Difference of Criteria

$$\mathsf{IC}_1 - \mathsf{IC}_0 = T\bar{Y}^2 - d_T$$

#### Selected Model

$$\widehat{M} = \left\{ \begin{array}{ll} \mathsf{M}_1, & |\sqrt{T}\,\bar{Y}| \geq \sqrt{d_T} \\ \mathsf{M}_0, & |\sqrt{T}\,\bar{Y}| \leq \sqrt{d_T} \end{array} \right.$$

## Case I: $\mu \neq 0$

Apply theory from earlier in lecture...

### KL-Divergence of M<sub>1</sub>

 $M_1$  is the true DGP with minimized KL-divergence equal to zero.

### KL-Divergence of M<sub>0</sub>

- ► Truth:  $g(y) = (2\pi)^{-1/2} \exp \left\{ -(y \mu)^2 / 2 \right\}$
- $M_0$ :  $f(y) = (2\pi)^{-1/2} \exp\{-y^2/2\}$
- Hence:  $\log g(y) \log f(y) = -\frac{1}{2}(y-\mu)^2 + \frac{1}{2}y^2 = \mu \left(y \frac{\mu}{2}\right)$

$$\begin{aligned} \mathsf{KL}(g;\mathsf{M}_0) &= \int_{\mathbb{R}} \mu(y - \mu/2) (2\pi)^{-1/2} \exp\left\{ (y - \mu)^2 / 2 \right\} \; \mathsf{d}y \\ &= \mu(\mu - \mu/2) = \mu^2 / 2 \end{aligned}$$

## Verifying Weak Consistency: $\mu \neq 0$

#### Condition on KL-Divergence

$$\liminf_{T \to \infty} \frac{1}{T} \sum_{t=1}^T \left\{ \textit{KL}(g; M_0) - \textit{KL}(g; M_1) \right\} = \liminf_{n \to \infty} \ \frac{1}{T} \sum_{t=1}^T \left( \frac{\mu^2}{2} - 0 \right) > 0$$

### Condition on Penalty

- ▶ Need  $c_{T,k} = o_p(T)$ , i.e.  $c_{T,k}/T \stackrel{p}{\rightarrow} 0$ .
- ▶ Both AIC and BIC satisfy this
- ▶ If  $\mu \neq 0$ , both AIC and BIC select M<sub>1</sub> wpa 1 as  $T \rightarrow \infty$ .

### Case II: $\mu = 0$

#### What's different?

- ▶ Both  $M_1$  and  $M_0$  are true and minimize KL divergence at zero.
- Consistency says choose most parsimonious true model: M<sub>0</sub>

### Verifying Conditions for Consistency

Use the second set of sufficient conditions:

- ▶ N(0,1) model nested inside  $N(\mu,1)$  model
- ▶ Truth is N(0,1) so LR-stat is asymptotically  $\chi^2(1) = O_p(1)$ .
- ▶ For penalty term, need  $\mathbb{P}(c_{T,k} c_{T,0}) \rightarrow \infty$
- BIC satisfies this but AIC doesn't.

## Finite-Sample Selection Probabilities: AIC

AIC Sets  $d_T = 2$ 

$$\widehat{M}_{AIC} = \left\{ \begin{array}{ll} M_1, & |\sqrt{T}\,\bar{Y}| \ge \sqrt{2} \\ M_0, & |\sqrt{T}\,\bar{Y}| < \sqrt{2} \end{array} \right.$$

$$\begin{split} P\left(\widehat{M}_{AIC} = M_1\right) &= P\left(\left|\sqrt{T}\,\bar{Y}\right| \geq \sqrt{2}\right) \\ &= P\left(\left|\sqrt{T}\,\mu + Z\right| \geq \sqrt{2}\right) \\ &= P\left(\sqrt{T}\,\mu + Z \leq -\sqrt{2}\right) + \left[1 - P\left(\sqrt{T}\,\mu + Z \leq \sqrt{2}\right)\right] \\ &= \Phi\left(-\sqrt{2} - \sqrt{T}\,\mu\right) + \left[1 - \Phi\left(\sqrt{2} - \sqrt{T}\,\mu\right)\right] \end{split}$$

where  $Z \sim N(0,1)$  since  $\bar{Y} \sim N(\mu, 1/T)$  because  $Var(Y_t) = 1$ .

## Finite-Sample Selection Probabilities: BIC

BIC sets  $d_T = \log(T)$ 

$$\widehat{M}_{BIC} = \left\{ \begin{array}{ll} M_1, & |\sqrt{T}\,\bar{Y}| \geq \sqrt{\log(T)} \\ M_0, & |\sqrt{T}\,\bar{Y}| < \sqrt{\log(T)} \end{array} \right.$$

Same steps as for the AIC except with  $\sqrt{\log(T)}$  in the place of  $\sqrt{2}$ :

$$\begin{split} P\left(\widehat{M}_{BIC} = M_1\right) &= P\left(\left|\sqrt{T}\,\bar{Y}\right| \geq \sqrt{\log(T)}\right) \\ &= \Phi\left(-\sqrt{\log(T)} - \sqrt{T}\mu\right) + \left[1 - \Phi\left(\sqrt{\log(T)} - \sqrt{T}\mu\right)\right] \end{split}$$

Interactive Demo: AIC vs BIC

https://fditraglia.shinyapps.io/CH\_Figure\_4\_1/

## Probability of Over-fitting

- ▶ If  $\mu = 0$  both models are true but  $M_0$  is more parsimonious.
- Probability of over-fitting (Z denotes standard normal):

$$P\left(\widehat{M} = M_1\right) = P\left(|\sqrt{T}\,\overline{Y}| \ge \sqrt{d_T}\right) = P(|Z| \ge \sqrt{d_T})$$
$$= P(Z^2 \ge d_T) = P(\chi_1^2 \ge d_T)$$

- AIC:  $d_T = 2$  and  $P(\chi_1^2 \ge 2) \approx 0.157$ .
- ▶ BIC:  $d_T = \log(T)$  and  $P(\chi_1^2 \ge \log T) \to 0$  as  $T \to 0$ .

AIC has  $\approx 16\%$  prob. of over-fitting; BIC does not over-fit in the limit.

### Risk of the Post-Selection Estimator

#### The Post-Selection Estimator

$$\widehat{\mu} = \left\{ \begin{array}{ll} \bar{Y}, & |\sqrt{T}\,\bar{Y}| \geq \sqrt{d_T} \\ 0, & |\sqrt{T}\,\bar{Y}| < \sqrt{d_T} \end{array} \right.$$

#### Recall from above

Recall from above that  $\sqrt{T}\bar{Y} = \sqrt{T}\mu + Z$  where  $Z \sim N(0,1)$ 

#### Risk Function

MSE risk times T since Var. of well-behaved estimator = O(1/T)

$$R_T(\mu) = T \cdot \mathbb{E}\left[(\widehat{\mu} - \mu)^2\right] = \mathbb{E}\left[\left(\sqrt{T}\widehat{\mu} - \sqrt{T}\mu\right)^2\right]$$

## Simplifying the MSE Risk Function

$$\sqrt{\mathit{T}}\,ar{\mathit{Y}} = \sqrt{\mathit{T}}\mu + \mathit{Z}$$
 where  $\mathit{Z} \sim \mathit{N}(0,1)$ 

Let 
$$X = \mathbf{1} \{A\}$$
 where  $A = \left\{ |\sqrt{T}\mu + Z| \ge \sqrt{d\tau} \right\}$ 

$$R_{T}(\mu) = \mathbb{E}\left[\left(\sqrt{T}\hat{\mu} - \sqrt{T}\mu\right)^{2}\right]$$

$$= \mathbb{E}\left\{\left[\left(\sqrt{T}\mu + Z\right)X - \sqrt{T}\mu\right]^{2}\right\}$$

$$= \mathbb{P}(A)\,\mathbb{E}\left\{\left[\left(\sqrt{T}\mu + Z\right) - \sqrt{T}\mu\right]^{2} \middle| X = 1\right\} + \left[1 - \mathbb{P}(A)\right]\left(\sqrt{T}\mu\right)^{2}$$

$$= \mathbb{P}(A)\,\mathbb{E}\left[Z^{2}|X = 1\right] + \left[1 - \mathbb{P}(A)\right]T\mu^{2}$$

So we need to calculate  $\mathbb{P}(A)$   $\mathbb{E}[Z^2|X=1]$  and  $\mathbb{P}(A)$ .

# Calculating $\mathbb{P}(A)$

Define 
$$a = (-\sqrt{d_T} - \sqrt{T}\mu)$$
 and  $b = (\sqrt{d_T} - \sqrt{T}\mu)$ 

$$\mathbb{P}(A) = \mathbb{P}\left(|\sqrt{T}\mu + Z| \ge \sqrt{d_T}\right)$$

$$= \mathbb{P}\left(\sqrt{T}\mu + Z \ge \sqrt{d_T}\right) + \mathbb{P}\left(\sqrt{T}\mu + Z \le -\sqrt{d_T}\right)$$

$$= \mathbb{P}(Z \ge b) + \mathbb{P}(Z \le a)$$

$$= 1 - \Phi(b) + \Phi(a)$$

And hence:

$$1 - \mathbb{P}(A) = \Phi(b) - \Phi(a)$$

# Calculating $\mathbb{P}(A)$ $\mathbb{E}[Z^2|X=1]$ – Step 1

Conditional Density of Z|X=1

$$f(z|x=1)=rac{\mathbf{1}(A)arphi(z)}{\mathbb{P}(A)}$$
 where  $arphi$  is the  $\mathit{N}(0,1)$  density

Therefore:

$$\mathbb{P}(A) \, \mathbb{E}[Z^2 | X = 1] = \mathbb{P}(A) \int_{\mathbb{R}} z^2 \left[ \frac{\mathbf{1}(A)\varphi(z)}{\mathbb{P}(A)} \right] \, \mathrm{d}z$$
$$= \int_{-\infty}^a z^2 \varphi(z) \, \mathrm{d}z + \int_b^\infty z^2 \varphi(z) \, \mathrm{d}z$$

# Calculating $\mathbb{P}(A)$ $\mathbb{E}[Z^2|X=1]$ – Step 2

Unconditional Expectation:  $\mathbb{E}[Z^2]$ 

$$1 = \mathbb{E}[Z^2] = \int_{-\infty}^a z^2 \varphi(z) \, \mathrm{d}z + \int_a^b z^2 \varphi(z) \, \mathrm{d}z + \int_b^\infty z^2 \varphi(z) \, \mathrm{d}z$$

Therefore:

$$\mathbb{P}(A) \, \mathbb{E}[Z^2 | X = 1] = \int_{-\infty}^a z^2 \varphi(z) \, \mathrm{d}z + \int_b^\infty z^2 \varphi(z) \, \mathrm{d}z$$
$$= 1 - \int_a^b z^2 \varphi(z) \, \mathrm{d}z$$

# Calculating $\mathbb{P}(A)$ $\mathbb{E}[Z^2|X=1]$ – Step 3

#### Integration By Parts

Take u = -z and  $dv = -z \exp\{-z^2/2\}$  since

$$\frac{d}{dz}\left(\exp\left\{-z^2/2\right\}\right) = -z\exp\left\{-z^2/2\right\}$$

Thus,  $v = \exp\{-z^2/2\}$ , du = -1 and

$$\int_{a}^{b} z^{2} \phi(z) dz = (2\pi)^{-1/2} \int_{a}^{b} z^{2} \exp\left\{-z^{2}/2\right\} dz$$

$$= (2\pi)^{-1/2} \left[ -z \exp\left\{-z^{2}/2\right\} \Big|_{a}^{b} + \int_{a}^{b} \exp\left\{-\frac{z^{2}}{2}\right\} dz \right]$$

$$= a\phi(a) - b\phi(b) + \Phi(b) - \Phi(a)$$

## The Simplifed MSE Risk Function

$$R_{T}(\mu) = 1 - [a\phi(a) - b\phi(b) + \Phi(b) - \Phi(a)] + T\mu^{2} [\Phi(b) - \Phi(a)]$$
$$= 1 + [b\phi(b) - a\phi(a)] + (T\mu^{2} - 1) [\Phi(b) - \Phi(a)]$$

where

$$a = -\sqrt{d_T} - \sqrt{T}\mu$$
$$b = \sqrt{d_T} - \sqrt{T}\mu$$

https://fditraglia.shinyapps.io/CH\_Figure\_4\_2/

### Punchline: Risk of the Post-Selection Estimator

- ► AIC: bounded worst-case risk
- ▶ BIC: low risk in a neighborhood of  $\mu = 0$  in exhange for unbounded worst-case risk as sample size grows
- General phenomenon: consistency and efficiency are mutually exclusive: consistent criteria have unbounded worst-case risk.

► For more details, see Yang (2007, ET)