

# 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 ( $AIC_c$ )

# Kullback-Leibler (KL) Divergence

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

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## Definition

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

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## Properties

- ▶ Not symmetric:  $\text{KL}(g; f) \neq \text{KL}(f; g)$
- ▶ By Jensen's Inequality:  $\text{KL}(g; f) \geq 0$  (strict iff  $g = f$  a.e.)
- ▶ Minimize KL  $\iff$  Maximize Expected log-likelihood

# KL Divergence and Mis-specified MLE

Pseudo-true Parameter Value  $\theta_0$

$$\hat{\theta}_{MLE} \xrightarrow{P} \theta_0 \equiv \arg \min_{\theta \in \Theta} \text{KL}(g; f_{\theta}) = \arg \max_{\theta \in \Theta} \mathbb{E}_G[\log f(Y|\theta)]$$

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

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Goal: Compare Mis-specified Models

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

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:  $Y_1, \dots, Y_n \sim \text{iid } g(y)$

Unbiased but Infeasible

$$\mathbb{E}_G \left[ \frac{1}{T} \ell(\theta_0) \right] = \mathbb{E}_G \left[ \frac{1}{T} \sum_{t=1}^T \log f(Y_t | \theta_0) \right] = \mathbb{E}_G [\log f(Y | \theta_0)]$$

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

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## Intuition for the Bias

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

# What to do about this bias?

1. General-purpose asymptotic approximation of “degree of over-optimism” of maximized sample log-likelihood.
  - ▶ Takeuchi's Information Criterion (TIC)
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## 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  $AIC_c$ .

# Recall: Asymptotics for Mis-specified ML Estimation

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

# Recall: Asymptotics for Mis-specified ML Estimation

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## Fundamental Expansion

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

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



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## Central Limit Theorem

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

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## Information Matrix Equality

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

# Bias Relative to Infeasible Plug-in Estimator

## Definition of Bias Term $B$

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

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## Question to Answer

On average, over the sampling distribution of  $\hat{\theta}$ , how large is  $B$ ?

AIC and TIC construct an asymptotic approximation of  $\mathbb{E}[B]$ .

# Derivation of AIC/TIC

## Step 1: Taylor Expansion

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

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

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## Derivation of AIC/TIC Continued...

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Step 4:  $U \sim N_p(0, K)$

$$\mathbb{E}[B] \approx \frac{1}{T}\mathbb{E}[U'J^{-1}U] = \frac{1}{T}\text{tr}\{J^{-1}K\}$$

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Final Result:

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

# TIC and AIC

## Takeuchi's Information Criterion

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

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## Akaike's Information Criterion

If  $g = f_{\theta}$  then  $J = K \Rightarrow \text{tr} \left\{ J^{-1} K \right\} = p \Rightarrow \text{AIC} = 2 \left[ \ell(\hat{\theta}) - p \right]$

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## 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,  $\ell(\hat{\theta})$  dominates.

# Corrected AIC ( $AIC_c$ ) – Hurvich & Tsai (1989)

## Idea Behind $AIC_c$

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

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Assumption: True DGP

$$\mathbf{y} = \mathbf{X}\beta_0 + \varepsilon, \quad \varepsilon \sim N(\mathbf{0}, \sigma_0^2 \mathbf{I}_T), \quad k \text{ Regressors}$$

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Can Show That

$$KL(g, f) = \frac{T}{2} \left[ \frac{\sigma_0^2}{\sigma_1^2} - \log \left( \frac{\sigma_0^2}{\sigma_1^2} \right) - 1 \right] + \left( \frac{1}{2\sigma_1^2} \right) (\beta_0 - \beta_1)' \mathbf{X}' \mathbf{X} (\beta_0 - \beta_1)$$

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?

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1. Would need to know  $(\beta_1, \sigma_1^2)$  for **candidate model**.
  - ▶ Easy: just use MLE  $(\hat{\beta}_1, \hat{\sigma}_1^2)$
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### Hurvich & Tsai (1989) Assume:

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

## Deriving the Corrected AIC

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

$$\widehat{KL} = \frac{T}{2} \left[ \frac{\sigma_0^2}{\hat{\sigma}^2} - \log \left( \frac{\sigma_0^2}{\hat{\sigma}^2} \right) - 1 \right] + \left( \frac{1}{2\hat{\sigma}^2} \right) (\hat{\beta} - \beta_0)' \mathbf{X}' \mathbf{X} (\hat{\beta} - \beta_0)$$

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

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

$$\text{AIC}_c = \log \hat{\sigma}^2 + \frac{T+k}{T-k-2}$$

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 $\mathbf{y}$ from $\mathbf{x}$ via Linear Regression

$$\underset{(T \times 1)}{\mathbf{y}} = \underset{(T \times K)}{\mathbf{X}} \underset{(K \times 1)}{\boldsymbol{\beta}} + \boldsymbol{\epsilon}$$

$$\mathbb{E}[\boldsymbol{\epsilon}|\mathbf{X}] = 0, \quad \text{Var}(\boldsymbol{\epsilon}|\mathbf{X}) = \sigma^2 \mathbf{I}$$

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- ▶ But  $\boldsymbol{\beta}$  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  $\beta$  is known.

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## Notation

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

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

Why not compare  $RSS(m)$ ?

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

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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.

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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 $\mathbf{X}\hat{\boldsymbol{\beta}}_m$ relative to infeasible optimum $\mathbf{X}\boldsymbol{\beta}$

Step 1: Algebra

$$\mathbf{X}\hat{\boldsymbol{\beta}}_m - \mathbf{X}\boldsymbol{\beta} = \mathbf{P}_m\mathbf{y} - \mathbf{X}\boldsymbol{\beta}$$



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

Step 1: Algebra

$$\begin{aligned}\mathbf{X}\hat{\boldsymbol{\beta}}_m - \mathbf{X}\boldsymbol{\beta} &= \mathbf{P}_m\mathbf{y} - \mathbf{X}\boldsymbol{\beta} = \mathbf{P}_m(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) - (\mathbf{I} - \mathbf{P}_m)\mathbf{X}\boldsymbol{\beta} \\ &= \mathbf{P}_m\boldsymbol{\epsilon} - (\mathbf{I} - \mathbf{P}_m)\mathbf{X}\boldsymbol{\beta}\end{aligned}$$

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

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Step 2:  $\mathbf{P}_m$  and  $(\mathbf{I} - \mathbf{P}_m)$  are symmetric, idempotent, and orthogonal

$$\left\| \mathbf{X}\hat{\boldsymbol{\beta}}_m - \mathbf{X}\boldsymbol{\beta} \right\|^2 = \{ \mathbf{P}_m\boldsymbol{\epsilon} - (\mathbf{I} - \mathbf{P}_m)\mathbf{X}\boldsymbol{\beta} \}' \{ \mathbf{P}_m\boldsymbol{\epsilon} + (\mathbf{I} - \mathbf{P}_m)\mathbf{X}\boldsymbol{\beta} \}$$

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

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Step 2:  $\mathbf{P}_m$  and  $(\mathbf{I} - \mathbf{P}_m)$  are symmetric, idempotent, and orthogonal

$$\begin{aligned}\left\|\mathbf{X}\hat{\boldsymbol{\beta}}_m - \mathbf{X}\boldsymbol{\beta}\right\|^2 &= \{\mathbf{P}_m\boldsymbol{\epsilon} - (\mathbf{I} - \mathbf{P}_m)\mathbf{X}\boldsymbol{\beta}\}' \{\mathbf{P}_m\boldsymbol{\epsilon} + (\mathbf{I} - \mathbf{P}_m)\mathbf{X}\boldsymbol{\beta}\} \\ &= \boldsymbol{\epsilon}'\mathbf{P}_m'\mathbf{P}_m\boldsymbol{\epsilon} - \boldsymbol{\beta}'\mathbf{X}'(\mathbf{I} - \mathbf{P}_m)'\mathbf{P}_m\boldsymbol{\epsilon} - \boldsymbol{\epsilon}'\mathbf{P}_m'(\mathbf{I} - \mathbf{P}_m)\mathbf{X}\boldsymbol{\beta} \\ &\quad + \boldsymbol{\beta}'\mathbf{X}'(\mathbf{I} - \mathbf{P}_m)(\mathbf{I} - \mathbf{P}_m)\mathbf{X}\boldsymbol{\beta}\end{aligned}$$

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

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Step 2:  $\mathbf{P}_m$  and  $(\mathbf{I} - \mathbf{P}_m)$  are symmetric, idempotent, and orthogonal

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# 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  $\mathbf{X}$

$$\begin{aligned}\text{MSE}(m|\mathbf{X}) &= \mathbb{E} \left[ (\mathbf{X}\hat{\boldsymbol{\beta}}_m - \mathbf{X}\boldsymbol{\beta})'(\mathbf{X}\hat{\boldsymbol{\beta}}_m - \mathbf{X}\boldsymbol{\beta}) | \mathbf{X} \right] \\ &= \mathbb{E} [\boldsymbol{\epsilon}'\mathbf{P}_m\boldsymbol{\epsilon} | \mathbf{X}] + \mathbb{E} [\boldsymbol{\beta}'\mathbf{X}'(\mathbf{I} - \mathbf{P}_m)\mathbf{X}\boldsymbol{\beta} | \mathbf{X}]\end{aligned}$$

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

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where  $k_m$  denotes the number of regressors in  $\mathbf{X}_m$  and

$$\text{tr}(\mathbf{P}_m) = \text{tr} \left\{ \mathbf{X}_m (\mathbf{X}_m' \mathbf{X}_m)^{-1} \mathbf{X}_m' \right\} = \text{tr} \left\{ \mathbf{X}_m' \mathbf{X}_m (\mathbf{X}_m' \mathbf{X}_m)^{-1} \right\} = \text{tr}(\mathbf{I}_m)$$

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

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

Bias-Variance Tradeoff

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### Bias-Variance Tradeoff

- ▶ Smaller Model  $\Rightarrow \sigma^2 k_m$  smaller: less estimation uncertainty.

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- ▶ 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.

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### Mallow's $C_p$

- ▶ Problem: MSE formula is infeasible since it involves  $\beta$  and  $\sigma^2$ .

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### 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.

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

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

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### 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  $\hat{\beta}$  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  $\hat{\beta}$  denote the full model estimator and  $\mathbf{P}$  be the corresponding projection matrix:  $\mathbf{X}\hat{\beta} = \mathbf{P}\mathbf{y}$ .

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

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### Crucial Fact

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

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## Step 4: Algebra using the preceding fact

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

Substituting  $\hat{\beta}$  doesn't work...

Step 5: Use “Trace Trick” on second term from Step 4

$$\mathbb{E}[\epsilon'(\mathbf{P} - \mathbf{P}_m)\epsilon | \mathbf{X}] = \mathbb{E}[\text{tr} \{ \epsilon'(\mathbf{P} - \mathbf{P}_m)\epsilon \} | \mathbf{X}]$$

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$$\begin{aligned}\mathbb{E}[\epsilon'(\mathbf{P} - \mathbf{P}_m)\epsilon|\mathbf{X}] &= \mathbb{E}[\text{tr}\{\epsilon'(\mathbf{P} - \mathbf{P}_m)\epsilon\}|\mathbf{X}] \\ &= \text{tr}\{\mathbb{E}[\epsilon\epsilon'|\mathbf{X}](\mathbf{P} - \mathbf{P}_m)\}\end{aligned}$$

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$$\begin{aligned}\mathbb{E}[\epsilon'(\mathbf{P} - \mathbf{P}_m)\epsilon|\mathbf{X}] &= \mathbb{E}[\text{tr}\{\epsilon'(\mathbf{P} - \mathbf{P}_m)\epsilon\}|\mathbf{X}] \\ &= \text{tr}\{\mathbb{E}[\epsilon\epsilon'|\mathbf{X}](\mathbf{P} - \mathbf{P}_m)\} \\ &= \text{tr}\{\sigma^2(\mathbf{P} - \mathbf{P}_m)\}\end{aligned}$$

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where  $K$  is the total number of regressors in  $\mathbf{X}$



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

Step 5: Use “Trace Trick” on second term from Step 4

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

where  $K$  is the total number of regressors in  $\mathbf{X}$

### Bias of Plug-in Estimator

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

## Putting Everything Together: Mallows's $C_p$

Want An Unbiased Estimator of This:

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

Previous Slide:

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

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

End Result:

$$\begin{aligned} \text{MC}(m) &= \hat{\sigma}^2 k_m + \left[ \hat{\boldsymbol{\beta}}' \mathbf{X}' (\mathbf{I} - \mathbf{P}_m) \mathbf{X} \hat{\boldsymbol{\beta}} - \hat{\sigma}^2 (K - k_m) \right] \\ &= \hat{\boldsymbol{\beta}}' \mathbf{X}' (\mathbf{I} - \mathbf{P}_m) \mathbf{X} \hat{\boldsymbol{\beta}} + \hat{\sigma}^2 (2k_m - K) \end{aligned}$$

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. . .

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

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Therefore:

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

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Just algebra, but tedious. . .

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

Therefore:

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

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

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

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

# Bayesian Model Comparison: Marginal Likelihoods

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

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

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

# Bayesian Model Comparison: Marginal Likelihoods

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

$$P(m|\mathbf{y}) = \frac{P(m)f(\mathbf{y}|m)}{f(\mathbf{y})} =$$



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

# Bayesian Model Comparison: Marginal Likelihoods

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## 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  $f(\mathbf{y})$  is constant across models.

# Laplace (aka Saddlepoint) Approximation

Suppress model index  $m$  for simplicity.

General Case: for  $T$  large...

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

$$p = \dim(\boldsymbol{\theta}), \quad \boldsymbol{\theta}_0 = \arg \max_{\boldsymbol{\theta} \in \Theta} h(\boldsymbol{\theta}), \quad H(\boldsymbol{\theta}_0) = -\frac{\partial^2 h(\boldsymbol{\theta})}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}'} \Big|_{\boldsymbol{\theta}=\boldsymbol{\theta}_0}$$

# Laplace (aka Saddlepoint) Approximation

Suppress model index  $m$  for simplicity.

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Use to Approximate Marginal Likelihood

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

and substitute  $\hat{\boldsymbol{\theta}}_{MLE}$  for  $\boldsymbol{\theta}_0$

# Laplace Approximation to Marginal Likelihood

Suppress model index  $m$  for simplicity.

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

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

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Take Logs and Multiply by 2

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

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The BIC

Assume uniform prior over **models** and ignore lower order terms:

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

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

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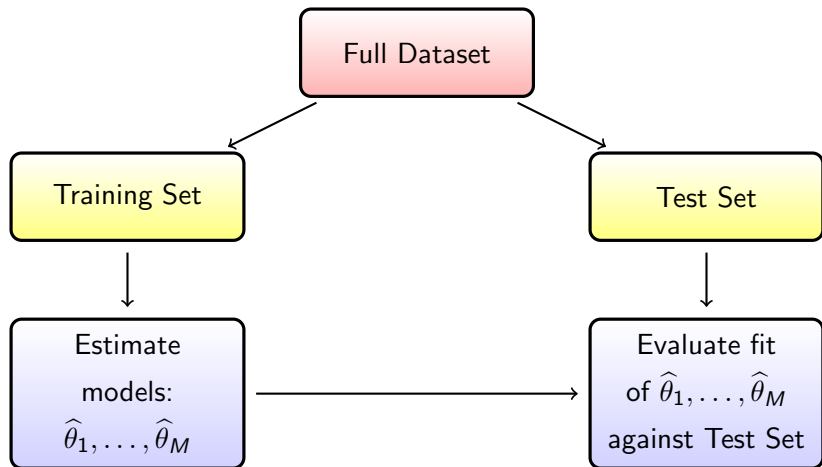
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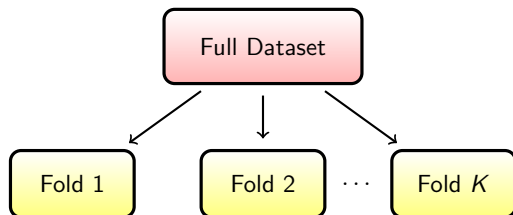
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- ▶ AIC/TIC,  $AIC_c$ , BIC,  $C_p$  **penalize** sample log-likelihood or RSS to compensate.
- ▶ Another idea: **don't re-use the same data!**

## 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.



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### 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!

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- ▶ 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  $Y_1, \dots, Y_T \sim \text{iid}$ . Let  $\hat{\theta}_{(t)}$  be the maximum likelihood estimator based on all observations **except**  $t$  and  $\hat{\theta}$  be the full-sample estimator.

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## Log-likelihood as “Loss”

$CV_1 = \frac{1}{T} \sum_{t=1}^T \log f(y_t | \hat{\theta}_{(t)})$  but since min. KL = max. log-like.  
we choose the model with **highest**  $CV_1(m)$ .

# Overview of the Proof

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

$$CV_1 = \frac{1}{T} \sum_{t=1}^T \log f(y_t | \hat{\theta}_{(t)})$$

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$$\begin{aligned} CV_1 &= \frac{1}{T} \sum_{t=1}^T \log f(y_t | \hat{\theta}_{(t)}) \\ &= \frac{1}{T} \sum_{t=1}^T \left[ \log f(y_t | \hat{\theta}) + \frac{\partial \log f(y_t | \hat{\theta})}{\partial \theta'} (\hat{\theta}_{(t)} - \hat{\theta}) \right] + o_p(1) \end{aligned}$$

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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:

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

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

$$\hat{J} = -\frac{1}{T} \sum_{t=1}^T \frac{\partial^2 \log f(y_t | \hat{\theta})}{\partial \theta \partial \theta'}$$

## Overview of Proof

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

$$-\frac{1}{T}\text{tr}\left\{\hat{J}^{-1}\hat{K}\right\} = -\frac{1}{T}\text{tr}\left\{\hat{J}^{-1}\left[\frac{1}{T}\sum_{t=1}^T\left(\frac{\partial \log f(y_t|\hat{\theta})}{\partial \theta}\right)\left(\frac{\partial \log f(y_t|\hat{\theta})}{\partial \theta}\right)'\right]\right\}$$

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So it suffices to show that

$$\left(\hat{\theta}_{(t)} - \hat{\theta}\right) = -\frac{1}{T}\hat{J}^{-1}\left[\frac{\partial\log f(y_t|\hat{\theta})}{\partial\theta}\right] + o_p(1)$$

# Digression: Functionals and Influence Functions

(Statistical) Functional

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## 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  $\mathbb{T}$ ?

$$\text{infl}(G, y) = \lim_{\epsilon \rightarrow 0} \frac{\mathbb{T}[(1 - \epsilon) G + \epsilon \delta_y] - \mathbb{T}(G)}{\epsilon}$$

## Back to the Proof...

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The influence function for ML estimation turns out to be

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### Step 3

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

$$\left(\hat{\theta}_{(t)} - \hat{\theta}\right) = -\frac{1}{T} \hat{J}^{-1} \left[ \frac{\partial \log f(y_t|\hat{\theta})}{\partial \theta} \right] + o_p(1)$$