

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

Motivation

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

Definition

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

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 θ_0

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

What if f_{θ} is correctly specified?

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

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 θ_0 is the pseudo-true parameter value for f_{θ} and γ_0 is the pseudo-true parameter value for h_{γ} .

How to Estimate Expected Log Likelihood?

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

Unbiased but Infeasible

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

Biased but Feasible

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

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)
 - ▶ Akaike’s Information Criterion (AIC)
2. Problem-specific finite sample approach, assuming $g \in f_\theta$.
 - ▶ Corrected AIC (AIC_c) 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_c .

Recall: Asymptotics for Mis-specified ML Estimation

Model $f(y|\theta)$, pseudo-true parameter θ_0 . For simplicity $Y_1, \dots, Y_T \sim \text{iid } g(y)$.

Fundamental Expansion

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

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

Central Limit Theorem

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

$$\sqrt{T}(\hat{\theta} - \theta_0) \rightarrow_d J^{-1} U \sim N_p(0, J^{-1} K J^{-1})$$

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

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

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

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

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

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

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

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

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

Derivation of AIC/TIC Continued...

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

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

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

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

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

Akaike's Information Criterion

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

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

Assumption: True DGP

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

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 (β_1, σ_1^2) that might not be the true parameters.

But how can we use this?

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

1. Would need to know (β_1, σ_1^2) for **candidate model**.
 - ▶ Easy: just use MLE $(\hat{\beta}_1, \hat{\sigma}_1^2)$
2. Would need to know (β_0, σ_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 $(\hat{\beta}, \hat{\sigma}^2)$ is consistent for truth.

Deriving the Corrected AIC

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

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

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

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

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

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

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

- ▶ If $\boldsymbol{\beta}$ were known, could never achieve lower MSE than by using all regressors to predict.
- ▶ 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 β is known.

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

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

Step 1: Algebra

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

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

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

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 \mathbf{X}

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

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

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

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

- ▶ 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 β and σ^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: $\mathbf{X}\hat{\beta} = \mathbf{P}\mathbf{y}$.

Crucial Fact

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

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

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

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:

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

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. . .

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

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 $m \in \mathcal{M}$

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

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...

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

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

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.

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

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

Bayesian Information Criterion

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

Take Logs and Multiply by 2

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

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

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_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.

Step 2

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

K -fold Cross-Validation: “Pseudo-out-of-sample”

Step 2

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

Step 3

Repeat Step 2 for each $k = 1, \dots, K$.

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 $CV_K = \frac{1}{T} \sum_{t=1}^T L(y_t, \hat{y}_t^{-k(t)})$ 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 \Rightarrow 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 $Y_1, \dots, Y_T \sim \text{iid}$. Let $\hat{\theta}_{(t)}$ be the maximum likelihood estimator based on all observations **except** t and $\hat{\theta}$ be the full-sample estimator.

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 $\hat{\theta}$:

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

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:

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

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

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

Example: ML Estimation

$$\theta_0 = \mathbb{T}(G) = \arg \min_{\theta \in \Theta} E_G \left[\log \left\{ \frac{g(Y)}{f(Y|\theta)} \right\} \right]$$

Influence Function

Let δ_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...

Step 1

The influence function for ML estimation turns out to be

$$\text{infl}(G, y) = J^{-1} \frac{\partial}{\partial \theta} \log f(y|\theta_0).$$

Step 2

Let \hat{G} denote the empirical CDF based on y_1, \dots, y_T . Then:

$$(\hat{\theta}_{(t)} - \hat{\theta}) = -\frac{1}{T} \text{infl}(\hat{G}, y_t) + o_p(1)$$

Step 3

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

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