Econ 722 – Advanced Econometrics IV, Part II

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Lecture #0 – Decision Theory

Statistical Decision Theory

The James-Stein Estimator

Decision Theoretic Preliminaries

Parameter $\theta \in \Theta$

Unknown state of nature, from parameter space Θ

Observed Data

Observe X with distribution F_θ from a sample space $\mathcal{X}$

Estimator $\widehat{\theta}$

An estimator (aka a decision rule) is a function from $\mathcal{X}$ to Θ

Loss Function $L(\theta, \widehat{\theta})$

A function from $\Theta \times \Theta$ to $\mathbb{R}$ that gives the cost we incur if we report $\widehat{\theta}$ when the true state of nature is θ.

Examples of Loss Functions

$L(\theta, \widehat{\theta}) = (\theta - \widehat{\theta})^2$	squared error loss
$L(\theta, \widehat{\theta}) = \lvert\theta - \widehat{\theta}\rvert$	absolute error loss
$L(\theta, \widehat{\theta}) = 0$ if $\theta = \widehat{\theta}$, 1 otherwise	zero-one loss
$L(\theta, \widehat{\theta}) = \int \log \left[\frac{f(x\mid\theta)}{f(x\mid\widehat{\theta})} \right] f(x\mid\theta)\, dx$	Kullback–Leibler loss

(Frequentist) Risk of an Estimator $\widehat{\theta}$

$$\boxed{R(\theta, \widehat{\theta}) = \mathbb{E}_\theta\left[L(\theta, \widehat{\theta})\right] = \int L\big(\theta, \widehat{\theta}(x)\big)\, dF_\theta(x)}$$

The frequentist decision theorist seeks to evaulate, for each θ, how much he would "expect" to lose if he used $\widehat{\theta}(X)$ repeatedly with varying X in the problem.

(Berger, 1985)

Example: Squared Error Loss

$$R(\theta, \widehat{\theta}) = \mathbb{E}_\theta\left[(\theta - \widehat{\theta})^2\right] = \mathsf{MSE} = \mathsf{Var}(\widehat{\theta}) + \mathsf{Bias}_\theta^2(\widehat{\theta})$$

Bayes Risk and Maximum Risk

Comparing Risk

$R(\theta, \widehat{\theta})$ is a *function* of θ rather than a single number. We want an estimator with low risk, but how can we compare?

Maximum Risk

$$\boxed{\bar{R}(\widehat{\theta}) = \sup_{\theta \in \Theta} R(\theta, \widehat{\theta})}$$

Bayes Risk

$$\boxed{r(\pi, \widehat{\theta}) = \mathbb{E}_{\pi}\left[R(\theta, \widehat{\theta})\right], \text{ where } \pi \text{ is a prior for } \theta}$$

Bayes and Minimax Rules

Minimize the Maximum or Bayes risk over all estimators $\widetilde{\theta}$

Minimax Rule/Estimator

$\widehat{\theta}$ is minimax if $\boxed{\sup_{\theta\in\Theta} R(\theta, \widehat{\theta}) = \inf_{\widetilde{\theta}} \sup_{\theta\in\Theta} R(\theta, \widetilde{\theta})}$

Bayes Rule/Estimator

$\widehat{\theta}$ is a Bayes rule with respect to prior π if $\boxed{r(\pi, \widehat{\theta}) = \inf_{\widetilde{\theta}} r(\pi, \widetilde{\theta})}$

Recall: Bayes' Theorem and Marginal Likelihood

Let π be a prior for θ. By Bayes' theorem, the posterior $\pi(\theta|\mathbf{x})$ is

$$\pi(\theta|\mathbf{x}) = \frac{f(\mathbf{x}|\theta)\pi(\theta)}{m(\mathbf{x})}$$

where the marginal likelihood $m(\mathbf{x})$ is given by

$$m(\mathbf{x}) = \int f(\mathbf{x}|\theta)\pi(\theta)\, d\theta$$

Posterior Expected Loss

Posterior Expected Loss

$$\rho\left(\pi(\theta|\mathbf{x}), \widehat{\theta}\,\right) = \int L\left(\theta, \widehat{\theta}\,\right)\pi(\theta|\mathbf{x})\, d\theta$$

Bayesian Decision Theory

Choose an estimator that minimizes posterior expected loss.

Easier Calculation

Since $m(\mathbf{x})$ does not depend on θ, to minimize $\rho\left(\pi(\theta|\mathbf{x}), \widehat{\theta}\,\right)$ it suffices to minimize $\int L(\theta, \widehat{\theta})f(\mathbf{x}|\theta)\pi(\theta)\, d\theta$.

Question

Is there a relationship between Bayes risk, $r(\pi, \widehat{\theta}) \equiv \mathbb{E}_\pi[R(\theta, \widehat{\theta})]$, and posterior expected loss?

Bayes Risk vs. Posterior Expected Loss

Theorem

$$r(\pi, \widehat{\theta}) = \int \rho\big(\pi(\theta|\mathbf{x}), \widehat{\theta}(\mathbf{x})\big)\, m(\mathbf{x})\, d\mathbf{x}$$

Proof

$$\begin{aligned}
r(\pi, \widehat{\theta}) &= \int R(\theta, \widehat{\theta})\pi(\theta)\, d\theta = \int \left[\int L\big(\theta, \widehat{\theta}(\mathbf{x})\big) f(\mathbf{x}|\theta)\, d\mathbf{x}\right] \pi(\theta)\, d\theta \\
&= \int \int L\big(\theta, \widehat{\theta}(\mathbf{x})\big) \left[f(\mathbf{x}|\theta)\pi(\theta)\right]\, d\mathbf{x} d\theta \\
&= \int \int L\big(\theta, \widehat{\theta}(\mathbf{x})\big) \left[\pi(\theta|\mathbf{x}) m(\mathbf{x})\right]\, d\mathbf{x} d\theta \\
&= \int \left[\int L\big(\theta, \widehat{\theta}(\mathbf{x})\big) \pi(\theta|\mathbf{x})\, d\theta\right] m(\mathbf{x})\, d\mathbf{x} \\
&= \int \rho\big(\pi(\theta|\mathbf{x}), \widehat{\theta}(\mathbf{x})\big)\, m(\mathbf{x})\, d\mathbf{x}
\end{aligned}$$

Finding a Bayes Estimator

Hard Problem

Find the function $\widehat{\theta}(\mathbf{x})$ that minimizes $r(\pi, \widehat{\theta})$.

Easy Problem

Find the number $\widehat{\theta}$ that minimizes $\rho\big(\pi(\theta|\mathbf{x}), \widehat{\theta}\big)$

Punchline

Since $r(\pi, \widehat{\theta}) = \int \rho\big(\pi(\theta|\mathbf{x}), \widehat{\theta}(\mathbf{x})\big)\, m(\mathbf{x})\, d\mathbf{x}$, to minimize $r(\pi, \widehat{\theta})$ we can set $\widehat{\theta}(\mathbf{x})$ to be the value $\widehat{\theta}$ that minimizes $\rho\big(\pi(\theta|\mathbf{x}), \widehat{\theta}\big)$.

Bayes Estimators for Common Loss Functions

Zero-one Loss

For zero-one loss, the Bayes estimator is the posterior mode.

Absolute Error Loss: $L(\theta, \widehat{\theta}) = |\theta - \widehat{\theta}|$

For absolute error loss, the Bayes estimator is the posterior median.

Squared Error Loss: $L(\theta, \widehat{\theta}) = (\theta - \widehat{\theta})^2$

For squared error loss, the Bayes estimator is the posterior mean.

Derivation of Bayes Estimator for Squared Error Loss

By definition,

$$\widehat{\theta} \equiv \underset{a \in \Theta}{\arg\min} \int (\theta - a)^2 \pi(\theta|\mathbf{x})\, d\theta$$

Differentiating with respect to a, we have

$$\begin{aligned} 2\int (\theta - a)\pi(\theta|\mathbf{x})\, d\theta &= 0 \\ \int \theta\pi(\theta|\mathbf{x})\, d\theta &= a \end{aligned}$$

Example: Bayes Estimator for a Normal Mean

Suppose $X \sim N(\mu, 1)$ and π is a $N(a, b^2)$ prior. Then,

$$\begin{aligned}
\pi(\mu|x) &\propto f(x|\mu) \times \pi(\mu) \\
&\propto \exp\left\{-\frac{1}{2}\left[(x-\mu)^2 + \frac{1}{b^2}(\mu - a)^2\right]\right\} \\
&\propto \exp\left\{-\frac{1}{2}\left[\left(1 + \frac{1}{b^2}\right)\mu^2 - 2\left(x + \frac{a}{b^2}\right)\mu\right]\right\} \\
&\propto \exp\left\{-\frac{1}{2}\left(\frac{b^2+1}{b^2}\right)\left[\mu - \left(\frac{b^2 x + a}{b^2+1}\right)\right]^2\right\}
\end{aligned}$$

So $\pi(\mu|x)$ is $N(m, \omega^2)$ with $\omega^2 = \frac{b^2}{1+b^2}$ and $m = \omega^2 x + (1-\omega^2)a$.

Hence the Bayes estimator for μ under squared error loss is

$$\boxed{\widehat{\theta}(X) = \frac{b^2 X + a}{1 + b^2}}$$

Minimax Analysis

Wasserman (2004)

The advantage of using maximum risk, despite its problems, is that it does not require one to choose a prior.

Berger (1986)

Perhaps the greatest use of the minimax principle is in situations for which no prior information is available . . . but two notes of caution should be sounded. First, the minimax principle can lead to bad decision rules. . . Second, the minimax approach can be devilishly hard to implement.

Methods for Finding a Minimax Estimator

1. Direct Calculation
2. Guess a "Least Favorable" Prior
3. Search for an "Equalizer Rule"

Method 1 rarely applicable so focus on 2 and 3...

Minimax Estimators and Least Favorable Priors

Theorem

Let $\widehat{\theta}$ be a Bayes rule with respect to π and suppose that for all $\theta \in \Theta$ we have $R(\theta, \widehat{\theta}) \leq r(\pi, \widehat{\theta})$. Then $\widehat{\theta}$ is a minimax estimator, and π is called a **least favorable prior**.

Proof

Suppose that $\widehat{\theta}$ is not minimax. Then there exists another estimator $\widetilde{\theta}$ with $\sup_{\theta \in \Theta} R(\theta, \widetilde{\theta}) < \sup_{\theta \in \Theta} R(\theta, \widehat{\theta})$. But since

$$r(\pi, \widetilde{\theta}) \equiv \mathbb{E}_\pi \left[R(\theta, \widetilde{\theta}) \right] \leq \mathbb{E}_\pi \left[\sup_{\theta \in \Theta} R(\theta, \widetilde{\theta}) \right] = \sup_{\theta \in \Theta} R(\theta, \widetilde{\theta})$$

but this implies that $\widehat{\theta}$ is *not* Bayes with respect to π since

$$r(\pi, \widetilde{\theta}) \leq \sup_{\theta \in \Theta} R(\theta, \widetilde{\theta}) < \sup_{\theta \in \Theta} R(\theta, \widehat{\theta}) \leq r(\pi, \widehat{\theta})$$

Try to use the preceding result to show that for the problem $X \sim N(\theta, 1)$ with squared error loss and $\Theta = [-m, m]$ for $0 < m < 1$ then the unique minimax estimator is $m \tanh(mX)$ and the least favorable prior puts $1/2$ probability on m and the rest on $-m$.

Equalizer Rules

Definition

An estimator $\widehat{\theta}$ is called an **equalizer rule** if its risk function is constant: $R(\theta, \widehat{\theta}) = C$ for some C.

Theorem

If $\widehat{\theta}$ is an equalizer rule and is Bayes with respect to π, then $\widehat{\theta}$ is minimax and π is least favorable.

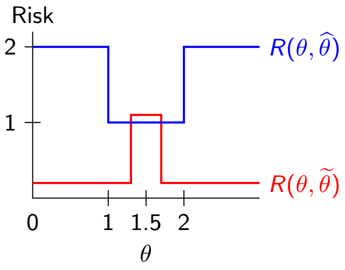
Proof

$$r(\pi, \widehat{\theta}) = \int R(\theta, \widehat{\theta})\pi(\theta)\, d\theta = \int C\pi(\theta)\, d\theta = C$$

Hence, $R(\theta, \widehat{\theta}) \leq r(\pi, \widehat{\theta})$ for all θ so we can apply the preceding theorem. Maybe take this out and assign it as homework?

Add an example. Possibly talk about generalized Bayes and sequences of priors.

Problems with the Minimax Principle



In the left panel, $\widetilde{\theta}$ is preferred by the minimax principle; in the right panel $\widehat{\theta}$ is preferred. But the only difference between them is that the right panel adds an additional *fixed* loss of 1 for $1 \leq \theta \leq 2$.

Problems with the Minimax Principle

Suppose that $\Theta = \{\theta_1, \theta_2\}$, $\mathcal{A} = \{a_1, a_2\}$ and the loss function is:

	a_1	a_2
θ_1	10	10.01
θ_2	8	-8

- Minimax principle: choose a_1
- Bayes: Choose a_2 unless $\pi(\theta_1) > 0.9994$

Minimax ignores the fact that under θ_1 we can never do better than a loss of 10, and tries to prevent us from incurring a tiny additional loss of 0.01

Regret and minimax regret. And maybe Gamma-minimax, and gamma-minimax regret.

Dominance and Admissibility

Dominance

$\widehat{\theta}$ **dominates** $\widetilde{\theta}$ with respect to R if $R(\theta, \widehat{\theta}) \leq R(theta, \widetilde{\theta})$ for all $\theta \in \Theta$ and the inequality is strict for at least one value of θ.

Admissibility

$\widehat{\theta}$ is **admissible** if no other estimator dominates it.

Inadmissiblility

$\widehat{\theta}$ is **inadmissible** if there is an estimator that dominates it.

Strong Inadmissibility

We say that $\widehat{\theta}$ is **strongly inadmissible** if there exists an estimator $\widetilde{\theta}$ and an $\varepsilon > 0$ such that $R(\theta, \widetilde{\theta}) < R(\theta, \widehat{\theta}) - \varepsilon$ for all θ.

Example of Admissible Estimator

Example

If $X \sim N(\theta, 1)$ then $\widehat{\theta}(X) = 3$ is admissible under squared error loss. FILL IN DETAILS

Bayes Rules are Admissible

Theorem A-1

Suppose that Θ is a discrete set and π gives strictly positive probability to each element of Θ. Then, if $\widehat{\theta}$ is a Bayes rule with respect to π, it is admissible.

Theorem A-2

If a Bayes rule is unique, it is admissible.

Theorem A-3

Suppose that $R(\theta, \widehat{\theta})$ is continuous in θ for all $\widehat{\theta}$ and that π gives strictly positive probability to any open subset of Θ. Then if $\widehat{\theta}$ is a Bayes rule with respect to π, it is admissible.

Add proof of one of the preceding theorems and assign the others for homework.

Admissibility and Minimax

Theorem

If $\widehat{\theta}$ has constant risk and is admissible, then it is minimax.

Theorem

If $\widehat{\theta}$ is minimax, then it is **not** strongly inadmissible.

Example

Sample mean unbounded parameter space is admissible (hard to prove this, but it's basically a limit of a Bayes rule) and constant risk (easy to see this), hence minimax

Possibly assign these for homework. I have a proof for the first, and the second seems straightforward.

Recall: Gauss-Markov Theorem

Linear Regression Model

$$\mathbf{y} = X\beta + \boldsymbol{\epsilon}, \quad \mathbb{E}[\boldsymbol{\epsilon}|X] = \mathbf{0}$$

Best Linear Unbiased Estimator

- $\text{Var}(\epsilon|X) = \sigma^2 I \Rightarrow$ then OLS has lowest variance among linear, unbiased estimators of β.
- $\text{Var}(\varepsilon|X) \neq \sigma^2 I \Rightarrow$ then GLS gives a lower variance estimator.

What if we consider biased estimators and squared error loss?

A Very Simple Example: $X \sim N(\theta, I)$

Goal

Estimate the p-vector θ using X with $L(\theta, \widehat{\theta}) = ||\widehat{\theta} - \theta||^2$.

Maximum Likelihood Estimator $\widehat{\theta}$

MLE $=$ sample mean, but only one observation: $\hat{\theta} = X$.

Risk of $\widehat{\theta}$

$$\left(\hat{\theta} - \theta\right)' \left(\hat{\theta} - \theta\right) = (X - \theta)' (X - \theta) = \sum_{i=1}^{p} (X_i - \theta_i)^2 \sim \chi^2_p$$

Since $\mathbb{E}[\chi^2_p] = p$, we have $R(\theta, \hat{\theta}) = p$.

A Very Simple Example: $X \sim N(\theta, I)$

James-Stein Estimator

$$\hat{\theta}^{JS} = \hat{\theta}\left(1 - \frac{p-2}{\hat{\theta}'\hat{\theta}}\right) = X - \frac{(p-2)\,X}{X'X}$$

- Shrinks components of sample mean vector towards zero
- More elements in $\theta \Rightarrow$ more shrinkage
- MLE close to zero ($\widehat{\theta}'\widehat{\theta}$ small) gives more shrinkage

MSE of James-Stein Estimator

$$
\begin{aligned}
R\left(\theta, \hat{\theta}^{JS}\right) &= \mathbb{E}\left[\left(\hat{\theta}^{JS} - \theta\right)'\left(\hat{\theta}^{JS} - \theta\right)\right] \\
&= \mathbb{E}\left[\left\{(X - \theta) - \frac{(p-2)X}{X'X}\right\}'\left\{(X - \theta) - \frac{(p-2)X}{X'X}\right\}\right] \\
&= \mathbb{E}\left[(X-\theta)'(X-\theta)\right] - 2(p-2)\mathbb{E}\left[\frac{X'(X-\theta)}{X'X}\right] \\
&\quad + (p-2)^2\,\mathbb{E}\left[\frac{1}{X'X}\right] \\
&= p - 2(p-2)\mathbb{E}\left[\frac{X'(X-\theta)}{X'X}\right] + (p-2)^2\,\mathbb{E}\left[\frac{1}{X'X}\right]
\end{aligned}
$$

Using fact that $R(\theta, \widehat{\theta}) = p$

Simplifying the Second Term

Writing Numerator as a Sum

$$\mathbb{E}\left[\frac{X'(X-\theta)}{X'X}\right] = \mathbb{E}\left[\frac{\sum_{i=1}^{p} X_i\left(X_i-\theta_i\right)}{X'X}\right] = \sum_{i=1}^{p}\mathbb{E}\left[\frac{X_i(X_i-\theta_i)}{X'X}\right]$$

For $i = 1, \ldots, p$

$$\mathbb{E}\left[\frac{X_i(X_i-\theta_i)}{X'X}\right] = \mathbb{E}\left[\frac{X'X - 2X_i^2}{(X'X)^2}\right]$$

Not obvious: integration by parts, expectation as a p-fold integral, $X \sim N(\theta, I)$

Combining

$$\begin{aligned}
\mathbb{E}\left[\frac{X'(X-\theta)}{X'X}\right] &= \sum_{i=1}^{p}\mathbb{E}\left[\frac{X'X-2X_i^2}{(X'X)^2}\right] = p\mathbb{E}\left[\frac{1}{X'X}\right] - 2\mathbb{E}\left[\frac{\sum_{i=1}^{p} X_i^2}{(X'X)^2}\right] \\
&= p\mathbb{E}\left[\frac{1}{X'X}\right] - 2\mathbb{E}\left[\frac{X'X}{(X'X)^2}\right] = (p-2)\,\mathbb{E}\left[\frac{1}{X'X}\right]
\end{aligned}$$

The MLE is Inadmissible when $p \geq 3$

$$
\begin{aligned}
R\left(\theta, \hat{\theta}^{JS}\right) &= p - 2(p-2)\left\{(p-2)\,\mathbb{E}\left[\frac{1}{X'X}\right]\right\} + (p-2)^2\,\mathbb{E}\left[\frac{1}{X'X}\right] \\
&= p - (p-2)^2\,\mathbb{E}\left[\frac{1}{X'X}\right]
\end{aligned}
$$

- $\mathbb{E}[1/(X'X)]$ exists and is positive whenever $p \geq 3$
- $(p-2)^2$ is always positive
- Hence, second term in the MSE expression is *negative*
- First term is MSE of the MLE

Therefore James-Stein strictly dominates MLE whenever $p \geq 3$!

James-Stein More Generally

- Our example was specific, but the result is general:
  - MLE is inadmissible under quadratic loss in regression model with at least three regressors.
  - Note, however, that this is MSE for the *full parameter vector*
- James-Stein estimator is also inadmissible!
  - Dominated by "positive-part" James-Stein estimator:

$$\widehat{\beta}^{JS} = \widehat{\beta}\left[1 - \frac{(p-2)\widehat{\sigma}^2}{\widehat{\beta}' X' X \widehat{\beta}}\right]_+$$

  - $\widehat{\beta} = \text{OLS}$, $(x)_+ = \max(x, 0)$, $\widehat{\sigma}^2 =$ usual OLS-based estimator
  - Stops us us from shrinking *past* zero to get a negative estimate for an element of β with a small OLS estimate.
  - Positive-part James-Stein isn't admissible either!

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

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

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

$$\widehat{\theta}_{MLE} \xrightarrow{p} \theta_0 \equiv \underset{\theta \in \Theta}{\arg\min}\, \text{KL}(g; f_\theta) = \underset{\theta \in \Theta}{\arg\max}\, \mathbb{E}_G[\log f(Y|\theta)]$$

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

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

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: $Y_1, \ldots, Y_n \sim$ 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?

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 $Y_1, \ldots, Y_T \sim$ iid $g(y)$.

Fundamental Expansion

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

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

Central Limit Theorem

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

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

Information Matrix Equality

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

Bias Relative to Infeasible Plug-in Estimator

Definition of Bias Term B

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

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

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

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:

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

Akaike's Information Criterion

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

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, $\ell(\widehat{\theta})$ 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

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

Can Show That

$$KL(g, f) = \frac{T}{2}\left[\frac{\sigma_0^2}{\sigma_1^2} - \log\left(\frac{\sigma_0^2}{\sigma_1^2}\right) - 1\right] + \left(\frac{1}{2\sigma_1^2}\right)(\boldsymbol{\beta}_0 - \boldsymbol{\beta}_1)'\mathbf{X}'\mathbf{X}(\boldsymbol{\beta}_0 - \boldsymbol{\beta}_1)$$

Where f is a normal regression model with parameters $(\boldsymbol{\beta}_1, \sigma_1^2)$ that might not be the true parameters.

But how can we use this?

$$KL(g,f) = \frac{T}{2}\left[\frac{\sigma_0^2}{\sigma_1^2} - \log\left(\frac{\sigma_0^2}{\sigma_1^2}\right) - 1\right] + \left(\frac{1}{2\sigma_1^2}\right)(\boldsymbol{\beta}_0 - \boldsymbol{\beta}_1)'\mathbf{X}'\mathbf{X}(\boldsymbol{\beta}_0 - \boldsymbol{\beta}_1)$$

1. Would need to know (β_1, σ_1^2) for candidate model.
   - Easy: just use MLE $(\widehat{\boldsymbol{\beta}}_1, \widehat{\sigma}_1^2)$
2. Would need to know $(\boldsymbol{\beta}_0, \sigma_0^2)$ 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 $(\widehat{\boldsymbol{\beta}}, \widehat{\sigma}^2)$ is consistent for truth.

Deriving the Corrected AIC

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

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

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

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

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

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

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 $\mathbf{y}$ 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 $\boldsymbol{\beta}$ is known.

Notation

- Model index m and regressor matrix $\mathbf{X}_m$
- Corresponding OLS estimator $\widehat{\boldsymbol{\beta}}_m$ 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: $\text{RSS}(m) = (\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}_m)'(\mathbf{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}_m)$

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 $\boldsymbol{X}\beta$

Step 1: Algebra

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

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

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

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

Step 3: Expectation of Step 2 conditional on $\mathbf{X}$

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

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

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

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

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 $\boldsymbol{\beta}$ and σ^2.
- Solution: Mallow's C_p constructs an unbiased estimator.
- Idea: what about plugging in $\widehat{\boldsymbol{\beta}}$ to estimate second term?

What if we plug in $\widehat{\boldsymbol{\beta}}$ 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 $\mathbf{P}$ be the corresponding projection matrix: $\mathbf{X}\widehat{\beta} = \mathbf{P}\mathbf{y}$.

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

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

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

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

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

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

Bias of Plug-in Estimator

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

Putting Everything Together: Mallow'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:

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

End Result:

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

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

Why is this different from the textbook formula?

Just algebra, but tedious...

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

Therefore:

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

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

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

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

Bayesian Model Comparison: Marginal Likelihoods

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

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

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

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

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

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…

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

$$p = \dim(\boldsymbol{\theta}), \;\; \boldsymbol{\theta}_0 = \arg\max_{\boldsymbol{\theta}\in\Theta} h(\boldsymbol{\theta}), \;\; H(\theta_0) = -\left.\frac{\partial^2 h(\boldsymbol{\theta})}{\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}'}\right|_{\boldsymbol{\theta}=\boldsymbol{\theta}_0}$$

Use to Approximate Marginal Likelihood

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

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

Laplace Approximation to Marginal Likelihood

Suppress model index m for simplicity.

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

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

Bayesian Information Criterion

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

Take Logs and Multiply by 2

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

The BIC

Assume uniform prior over models and ignore lower order terms:

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

large-sample Frequentist approx. to Bayesian marginal likelihood

Lecture #3 – Cross-Validation

Model selection via a Hold-out Sample

K-fold Cross-validation

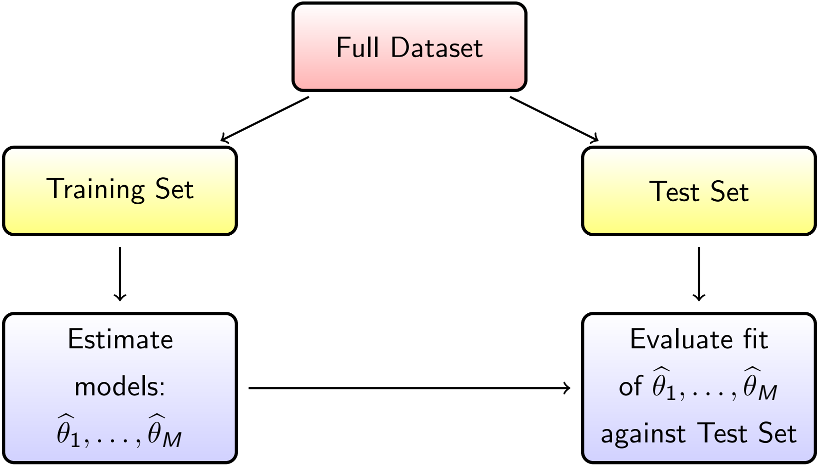
Asymptotic Equivalence Between LOO-CV and TIC

Influence Functions

Model Selection using a Hold-out Sample

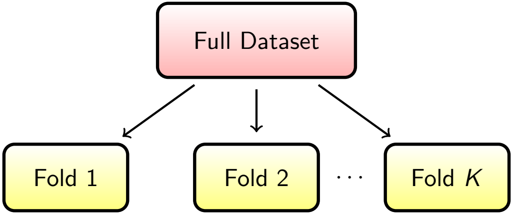
- The real problem is double use of the data: first for estimation, then for model comparison.
  - Maximized sample log-likelihood is an overly optimistic estimate of expected log-likelihood and hence KL-divergence
  - In-sample squared prediction error is an overly optimistic estimator of out-of-sample squared prediction error
- AIC/TIC, AIC_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 $\widehat{\theta}(-k)$.

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 $\widehat{\theta}(-k)$.

Step 3

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

Step 4

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

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

Step 4

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

Step 5

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

Step 5

Repeat for each model & choose m to minimize $\text{CV}_K(m)$.

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 $Y_1, \ldots, Y_T \sim$ 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"

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

Overview of the Proof

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

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

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:

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

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

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

Overview of Proof

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

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

So it suffices to show that

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

Digression: Functionals and Influence Functions

(Statistical) Functional

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

Example: ML Estimation

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

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 $\mathbb{T}$?

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

Back to the Proof...

Step 1

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

Step 2

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

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

Step 3

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

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