Econ 722 – Advanced Econometrics IV

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Lecture #1 – 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
$L(\theta, \widehat{\theta}) = \int \log \left[\frac{f(x\|\theta)}{f(x\|\widehat{\theta})} \right] f(x\|\theta)\, dx$	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

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

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,

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

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...

The Bayes Rule for a Least Favorable Prior is Minimax

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

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

Example of Least Favorable Prior

Bounded Normal Mean

- $X \sim N(\theta, 1)$
- Squared error loss
- $\Theta = [-m, m]$ for $0 < m < 1$

Least Favorable Prior

$\pi(\theta) = 1/2$ for $\theta \in \{-m, m\}$, zero otherwise.

Resulting Bayes Rule is Minimax

$$\widehat{\theta}(X) = m \tanh(mX) = m \left[\frac{\exp\{mX\} - \exp\{-mX\}}{\exp\{mX\} + \exp\{-mX\}}\right]$$

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.

Example: $X_1, \ldots, X_n \sim$ iid Bernoulli(p)

Under a Beta(α, β) prior with $\alpha = \beta = \sqrt{n}/2$,

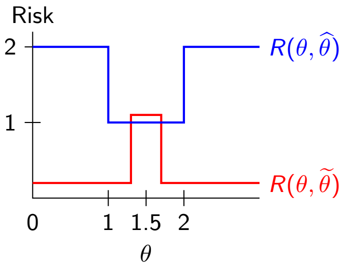
$$\widehat{p} = \frac{n\bar{X} + \sqrt{n}/2}{n + \sqrt{n}}$$

is the Bayesian posterior mean, hence the Bayes rule under squared error loss. The risk function of $\widehat{p}$ is,

$$R(p, \widehat{p}) = \frac{n}{4(n + \sqrt{n})^2}$$

which is constant in p. Hence, $\widehat{p}$ is an equalizer rule, and by the preceding theorem is minimax.

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

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.

Example of an Admissible Estimator

Say we want to estimate θ from $X \sim N(\theta, 1)$ under squared error loss. Is the estimator $\widehat{\theta}(X) = 3$ admissible?

If not, then there is a $\widetilde{\theta}$ with $R(\theta, \widetilde{\theta}) \leq R(\theta, \widehat{\theta})$ for all θ. Hence:

$$R(3, \widetilde{\theta}) \leq R(3, \widehat{\theta}) = \left\{\mathbb{E}\left[\widehat{\theta} - 3\right]\right\}^2 + \mathrm{Var}(\widehat{\theta}) = 0$$

Since R cannot be negative for squared error loss,

$$0 = R(3, \widetilde{\theta}) = \left\{\mathbb{E}\left[\widetilde{\theta} - 3\right]\right\}^2 + \mathrm{Var}(\widetilde{\theta})$$

Therefore $\widehat{\theta} = \widetilde{\theta}$, so $\widehat{\theta}$ is admissible, although very silly!

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.

Admissible Equalizer Rules are Minimax

Theorem

Let $\widehat{\theta}$ be an equalizer rule. Then if $\widehat{\theta}$ is admissible, it is minimax.

Proof

Since $\widehat{\theta}$ is an equalizer rule, $R(\theta, \widehat{\theta}) = C$. Suppose that $\widehat{\theta}$ is not minimax. Then there is a $\widetilde{\theta}$ such that

$$\sup_{\theta \in \Theta} R(\theta, \widetilde{\theta}) < \sup_{\theta \in \Theta} R(\theta, \widehat{\theta}) = C$$

But for any θ, $R(\theta, \widetilde{\theta}) \leq \sup_{\theta \in \Theta} R(\theta, \widetilde{\theta})$. Thus we have shown that $\widetilde{\theta}$ dominates $\widehat{\theta}$, so that $\widehat{\theta}$ cannot be admissible.

Minimax Implies "Nearly" Admissible

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.

Theorem

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

Example: Sample Mean, Unbounded Parameter Space

Theorem

Suppose that $X_1, \ldots, X_n \sim N(\theta, 1)$ with $\Theta = \mathbb{R}$. Under squared error loss, one can show that $\widehat{\theta} = \bar{X}$ is admissible.

Intuition

The proof is complicated, but effectively we view this estimator as a **limit** of a of Bayes estimator with prior $N(a, b^2)$, as $b^2 \to \infty$.

Minimaxity

Since $R(\theta, \bar{X}) = \mathrm{Var}(\bar{X}) = 1/n$, we see that $\bar{X}$ is an equalizer rule. Since it is admissible, it is therefore minimax.

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?

Multiple Normal Means: $X \sim N(\theta, I)$

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 $R(\theta, \hat{\theta}) = p$.

Multiple Normal Means: $X \sim N(\theta, I)$

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

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

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:

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

  - $\widehat{\beta} =$ 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 #2 – Model Selection I

Kullback-Leibler Divergence

Bias of Maximized Sample Log-Likelihood

Review of Asymptotics for Mis-specified MLE

Deriving AIC and TIC

Corrected AIC (AIC_c)

Mallow's C_p

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

$\text{KL}(g; f) \geq 0$ with equality iff $g = f$ almost surely

Jensen's Inequality

If φ is convex, then $\varphi(\mathbb{E}[X]) \leq \mathbb{E}[\varphi(X)]$, with strict equality when φ is affine or X is constant.

log is concave so $(-\log)$ is convex

$$
\begin{aligned}
\mathbb{E}_G\left[\log\left\{\frac{g(Y)}{f(Y)}\right\}\right] &= \mathbb{E}_G\left[-\log\left\{\frac{f(Y)}{g(Y)}\right\}\right] \geq -\log\left\{\mathbb{E}_G\left[\frac{f(Y)}{g(Y)}\right]\right\} \\
&= -\log\left\{\int_{-\infty}^{\infty} \frac{f(y)}{g(y)} \cdot g(y)\, dy\right\} \\
&= -\log\left\{\int_{-\infty}^{\infty} f(y)\, dy\right\} \\
&= -\log(1) = 0
\end{aligned}
$$

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

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
- $\mathbf{X}\widehat{\boldsymbol{\beta}}_m = \mathbf{X}_{(-m)}\mathbf{0} + \mathbf{X}_m\left[(\mathbf{X}_m'\mathbf{X}_m)^{-1}\mathbf{X}_m'\right]\mathbf{y} = \mathbf{P}_m\mathbf{y}$

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 both symmetric and idempotent, and orthogonal to each other

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

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

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

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

Step 4: Algebra using the preceding fact

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

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

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

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

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

Bias of Plug-in Estimator

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

Putting Everything Together: Mallow's C_p

Want An Unbiased Estimator of This:

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

Previous Slide:

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

End Result:

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

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...

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

Therefore:

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

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

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

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

Lecture #3 – Model Selection II

Bayesian Model Comparison

Bayesian Information Criterion (BIC)

K-fold Cross-validation

Asymptotic Equivalence Between LOO-CV and TIC

Bayesian Model Comparison: Marginal Likelihoods

Bayes' Theorem 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. . .

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

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

Use to Approximate Marginal Likelihood

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

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

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

Take Logs and Multiply by 2

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

The BIC

Assume uniform prior over models and ignore lower order terms:

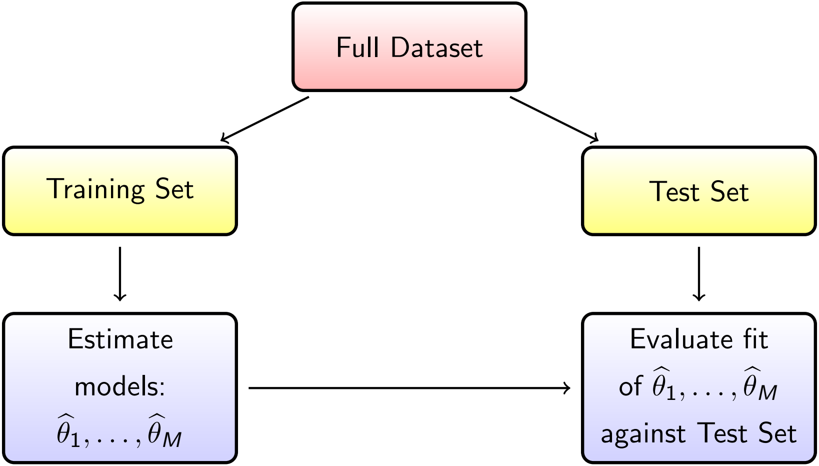
$$\text{BIC}(m) = 2\log f(\mathbf{y}|\widehat{\boldsymbol{\theta}}, m) - p_m \log(T)$$

large-sample Frequentist approx. to Bayesian marginal likelihood

Model Selection using a Hold-out Sample

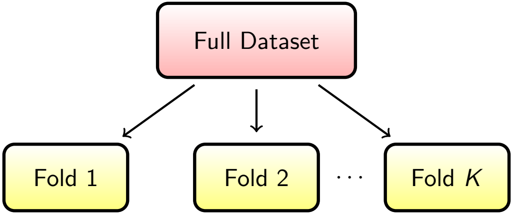
- The real problem is double use of the data: first for estimation, then for model comparison.
  - Maximized sample log-likelihood is an overly optimistic estimate of expected log-likelihood and hence KL-divergence
  - In-sample squared prediction error is an overly optimistic estimator of out-of-sample 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 $\log f\left(y_t|\widehat{\theta}_{(t)}\right)$ around $\widehat{\theta}$:

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

Why isn't the first-order term zero in this case?

Important Side Point

Definition of ML Estimator

$$\frac{\partial \ell(\widehat{\theta})}{\partial \theta'} = \frac{1}{T}\sum_{t=1}^{T} \frac{\partial \log f(y_t|\widehat{\theta})}{\partial \theta} = 0$$

In Contrast

$$\begin{aligned}\frac{1}{T}\sum_{t=1}^{T} \frac{\partial \log f(y_t|\widehat{\theta})}{\partial \theta'}\left(\widehat{\theta}_{(t)} - \widehat{\theta}\right) &= \left[\frac{1}{T}\sum_{t=1}^{T} \frac{\partial \log f(y_t|\widehat{\theta})}{\partial \theta'}\widehat{\theta}_{(t)}\right] - \widehat{\theta}\left[\frac{1}{T}\sum_{t=1}^{T} \frac{\partial \log f(y_t|\widehat{\theta})}{\partial \theta'}\right] \\ &= \frac{1}{T}\sum_{t=1}^{T} \frac{\partial \log f(y_t|\widehat{\theta})}{\partial \theta'}\widehat{\theta}_{(t)} \neq 0\end{aligned}$$

Overview of Proof

From expansion two slides back, 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

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

What is an Influence Function?

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 the CDF of a point mass at y: $\delta_y(a) = \mathbb{1}\{y \leq a\}$.

Influence function = functional derivative: how does a small change in G affect $\mathbb{T}$?

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

Relating Influence Functions to $\widehat{\theta}_{(t)}$

Empirical CDF $\widehat{G}$

$$\widehat{G}(a) = \frac{1}{T}\sum_{t=1}^{T} \mathbb{1}\left\{y_t \leq a\right\} = \frac{1}{T}\sum_{t=1}^{T}\delta_{y_t}(a)$$

Relation to "LOO" Empirical CDF $\widehat{G}_{(t)}$

$$\widehat{G} = \left(1 - \frac{1}{T}\right)\widehat{G}_{(t)} + \frac{\delta_{y_t}}{T}$$

Applying $\mathbb{T}$ to both sides…

$$\mathbb{T}(\widehat{G}) = \mathbb{T}\left((1 - 1/T)\widehat{G}_{(t)} + \delta_{y_t}/T\right)$$

Relating Influence Functions to $\widehat{\theta}_{(t)}$

Some algebra, followed by taking $\varepsilon = 1/T$ to zero gives:

$$\begin{aligned}
\mathbb{T}(\widehat{G}) &= \mathbb{T}\left((1-1/T)\widehat{G}_{(t)} + \delta_{y_t}/T\right) \\
\mathbb{T}(\widehat{G}) - \mathbb{T}(\widehat{G}_{(t)}) &= \mathbb{T}\left((1-1/T)\widehat{G}_{(t)} + \delta_{y_t}/T\right) - \mathbb{T}(\widehat{G}_{(t)}) \\
\mathbb{T}(\widehat{G}) - \mathbb{T}(\widehat{G}_{(t)}) &= \frac{1}{T}\left[\frac{\mathbb{T}\left((1-1/T)\widehat{G}_{(t)} + \delta_{y_t}/T\right) - \mathbb{T}(\widehat{G}_{(t)})}{1/T}\right] \\
\mathbb{T}(\widehat{G}) - \mathbb{T}(\widehat{G}_{(t)}) &= \frac{1}{T}\text{infl}\left(\widehat{G}_{(t)}, y_t\right) + o_p(1) \\
\widehat{\theta} - \widehat{\theta}_{(t)} &= \frac{1}{T}\text{infl}\left(\widehat{G}, y_t\right) + o_p(1)
\end{aligned}$$

Last step: difference between having $\widehat{G}$ vs. $\widehat{G}_{(t)}$ in infl is negligible

Steps for Last part of TIC/LOO-CV Equivalence Proof

Step 1

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 2

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

Step 3

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

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

Lecture #4 – Asymptotic Properties

Overview

Weak Consistency

Consistency

Efficiency

AIC versus BIC in a Simple Example

Overview

Asymptotic Properties

What happens as the sample size increases?

Consistency

Choose "best" model with probability approaching 1 in the limit.

Efficiency

Post-model selection estimator with low risk.

Some References

Sin and White (1992, 1996), Pötscher (1991), Leeb & Pötscher (2005), Yang (2005) and Yang (2007).

Penalizing the Likelihood

Examples we've seen:

$$\begin{aligned} TIC &= 2\ell_T(\widehat{\theta}) - 2\text{trace}\left\{\widehat{J}^{-1}\widehat{K}\right\} \\ AIC &= 2\ell_T(\widehat{\theta}) - 2\ \text{length}(\theta) \\ BIC &= 2\ell_T(\widehat{\theta}) - \log(T)\ \text{length}(\theta) \end{aligned}$$

Generic penalty $c_{T,k}$

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

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

Weak Consistency: Suppose M_{k_0} Uniquely Minimizes KL

Assumption

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

Consequences

- Any criterion with $c_{T,k}>0$ and $c_{T,k}=o_p(T)$ is weakly consistent: selects M_{k_0} wpa 1 in the limit.
- Weak consistency still holds if $c_{T,k}$ is zero for one of the models, so long as it is strictly positive for all the others.

Both AIC and BIC are Weakly Consistent

Both satisfy $T^{-1} c_{T,k} \xrightarrow{p} 0$.

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

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

Consistency: No Unique KL-minimizer

Example

If the truth is an AR(5) model then AR(6), AR(7), AR(8), etc. models all have zero KL-divergence.

Principle of Parsimony

Among the KL-minimizers, choose the simplest model, i.e. the one with the fewest parameters.

Notation

$\mathcal{J} =$ be the set of all models that attain minimum KL-divergence

$\mathcal{J}_0 =$ subset with the minimum number of parameters.

Sufficient Conditions for Consistency

Consistency: Select Model from $\mathcal{J}_0$ wpa 1

$$\lim_{T\to\infty} \mathbb{P}\left\{\min_{\ell\in\mathcal{J}\setminus\mathcal{J}_0} \left[IC(M_{j_0}) - IC(M_\ell)\right] > 0\right\} = 1$$

Sufficient Conditions

(i) For all $k \neq \ell \in \mathcal{J}$

$$\sum_{t=1}^{T} \left[\log f_{k,t}(Y_t|\theta_k^*) - \log f_{\ell,t}(Y_t|\theta_\ell^*)\right] = O_p(1)$$

where θ_k^* and θ_ℓ^* are the KL minimizing parameter values.

(ii) For all $j_0 \in \mathcal{J}_0$ and $\ell \in (\mathcal{J}\setminus\mathcal{J}_0)$

$$P\left(c_{T,\ell} - c_{T,j_0} \to \infty\right) = 1$$

BIC is Consistent; AIC and TIC Are Not

- AIC and TIC *cannot* satisfy (ii) since $(c_{T,\ell} - c_{T,j_0})$ *does not depend on sample size*.
- It turns out that AIC and TIC are *not* consistent.
- BIC is consistent:

$$c_{T,\ell} - c_{T,j_0} = \log(T)\left\{\text{length}(\theta_\ell) - \text{length}(\theta_{j_0})\right\}$$

- Term in braces is *positive* since $\ell \in \mathcal{J} \backslash \mathcal{J}_0$, i.e. ℓ is not as parsimonious as j_0
- $\log(T) \to \infty$, so BIC always selects a model in $\mathcal{J}_0$ in the limit.

Efficiency: Risk Properties of Post-selection Estimator

Setup

- Models M_0 and M_1; corresponding estimators $\widehat{\theta}_{0,T}$ and $\widehat{\theta}_{1,T}$
- Model Selection: If $\widehat{M} = 0$ choose M_0; if $\widehat{M} = 1$ choose M_1.

Post-selection Estimator

$$\widehat{\theta}_{\widehat{M},T} \equiv \mathbf{1}_{\{\widehat{M}=0\}}\widehat{\theta}_{0,T} + \mathbf{1}_{\{\widehat{M}=1\}}\widehat{\theta}_{1,T}$$

Two Sources of Randomness

Variability in $\widehat{\theta}_{\widehat{M},T}$ arises both from $\left(\widehat{\theta}_{0,T}, \widehat{\theta}_{1,T}\right)$ and from $\widehat{M}$.

Question

How does the risk of $\widehat{\theta}_{\widehat{M},T}$ compare to that of other estimators?

Efficiency: Risk Properties of Post-selection Estimator

Pointwise-risk Adaptivity

$\widehat{\theta}_{\widehat{M},T}$ is **pointwise-risk adaptive** if for any fixed $\theta \in \Theta$,

$$\frac{R(\theta, \widehat{\theta}_{\widehat{M},T})}{\min\left\{R(\theta, \widehat{\theta}_{0,T}),\ R(\theta, \widehat{\theta}_{1,T})\right\}} \to 1, \quad \text{as } T \to \infty$$

Minimax-rate Adaptivity

$\widehat{\theta}_{\widehat{M},T}$ is **minimax-rate adaptive** if

$$\sup_T \left[\frac{\sup_{\theta \in \Theta} R(\theta, \widehat{\theta}_{\widehat{M},T})}{\inf_{\widetilde{\theta}_T} \sup_{\theta \in \Theta} R(\theta, \widetilde{\theta}_T)} \right] < \infty$$

The Strengths of AIC and BIC Cannot be Shared

Theorem

No model post-model selection estimator can be both pointwise-risk adaptive and minimax-rate adaptive.

AIC vs. BIC

- BIC is pointwise-risk adaptive but AIC is not. (This is effectively identical to consistency.)
- AIC is minimax-rate adaptive, but BIC is not.
- Further Reading: Yang (2005), Yang (2007)

Consistency and Efficiency in a Simple Example

Information Criteria

Consider criteria of the form $\mathrm{IC}_m = 2\ell(\theta) - d_T \times \mathrm{length}(\theta)$.

True DGP

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

Candidate Models

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

$$\mathrm{IC}_0 = 2 \max_{\mu} \{\ell(\mu) \colon \mathrm{M}_0\}$$

$$\mathrm{IC}_1 = 2 \max_{\mu} \{\ell(\mu) \colon \mathrm{M}_1\} - d_T$$

Log-Likelihood Function

Simple Algebra

$$\ell_T(\mu) = \text{Constant} - \frac{1}{2}\sum_{t=1}^{T}(Y_t - \mu)^2$$

Tedious Algebra

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

Combining These

$$\ell_T(\mu) = \text{Constant} - \frac{T}{2}\left(\bar{Y} - \mu\right)^2$$

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

Information Criteria

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

$$\mathrm{IC}_0 = 2 \max_{\mu} \{\ell(\mu)\colon \mathrm{M}_0\} = 2 \times \text{Constant} - T\bar{Y}^2$$

$$\mathrm{IC}_1 = 2 \max_{\mu} \{\ell(\mu)\colon \mathrm{M}_1\} - d_T = 2 \times \text{Constant} - d_T$$

Difference of Criteria

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

Selected Model

$$\widehat{\mathrm{M}} = \begin{cases} \mathrm{M}_1, & |\sqrt{T}\bar{Y}| \geq \sqrt{d_T} \\ \mathrm{M}_0, & |\sqrt{T}\bar{Y}| < \sqrt{d_T} \end{cases}$$

Verifying Weak Consistency: $\mu \neq 0$

KL Divergence for M_0 and M_1

$KL(g; M_0) = \mu^2/2, \quad KL(g; M_1) = 0$

Condition on KL-Divergence

$$\liminf_{T\to\infty} \frac{1}{T}\sum_{t=1}^{T}\left\{KL(g;\mathrm{M}_0) - KL(g;\mathrm{M}_1)\right\} = \liminf_{T\to\infty} \frac{1}{T}\sum_{t=1}^{T}\left(\frac{\mu^2}{2} - 0\right) > 0$$

Condition on Penalty

- Need $c_{T,k} = o_p(T)$, i.e. $c_{T,k}/T \xrightarrow{p} 0$.
- Both AIC and BIC satisfy this
- If $\mu \neq 0$, both AIC and BIC select M_1 wpa 1 as $T \to \infty$.

Verifying Consistency: $\mu = 0$

What's different?

- Both M_1 and M_0 are true and minimize KL divergence at zero.
- Consistency says choose most parsimonious true model: M_0

Verifying Conditions for Consistency

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

Finite-Sample Selection Probabilities: AIC

AIC Sets $d_T = 2$

$$\widehat{M}_{AIC} = \begin{cases} M_1, & |\sqrt{T}\bar{Y}| \geq \sqrt{2} \\ M_0, & |\sqrt{T}\bar{Y}| < \sqrt{2} \end{cases}$$

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

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

Finite-Sample Selection Probabilities: BIC

BIC sets $d_T = \log(T)$

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

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

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

Interactive Demo: AIC vs BIC

`https://fditraglia.shinyapps.io/CH_Figure_4_1/`

Probability of Over-fitting

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

$$\begin{aligned} P\left(\widehat{M} = M_1\right) &= P\left(|\sqrt{T}\bar{Y}| \geq \sqrt{d_T}\right) = P(|Z| \geq \sqrt{d_T}) \\ &= P(Z^2 \geq d_T) = P(\chi^2_1 \geq d_T) \end{aligned}$$

- AIC: $d_T = 2$ and $P(\chi^2_1 \geq 2) \approx 0.157$.
- BIC: $d_T = \log(T)$ and $P(\chi^2_1 \geq \log T) \to 0$ as $T \to \infty$.

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

Risk of the Post-Selection Estimator

The Post-Selection Estimator

$$\widehat{\mu} = \begin{cases} \bar{Y}, & |\sqrt{T}\bar{Y}| \geq \sqrt{d_T} \\ 0, & |\sqrt{T}\bar{Y}| < \sqrt{d_T} \end{cases}$$

Recall from above

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

Risk Function

MSE risk times T to get risk relative to minimax rate: $1/T$.

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

The Simplifed MSE Risk Function

$$
\begin{aligned}
R(\mu, \widehat{\mu}) &= 1 - \left[a\phi(a) - b\phi(b) + \Phi(b) - \Phi(a)\right] + T\mu^2 \left[\Phi(b) - \Phi(a)\right] \\
&= 1 + \left[b\phi(b) - a\phi(a)\right] + \left(T\mu^2 - 1\right)\left[\Phi(b) - \Phi(a)\right]
\end{aligned}
$$

where

$$
\begin{aligned}
a &= -\sqrt{d_T} - \sqrt{T}\mu \\
b &= \sqrt{d_T} - \sqrt{T}\mu
\end{aligned}
$$

`https://fditraglia.shinyapps.io/CH_Figure_4_2/`

Understanding the Risk Plot

AIC

- For any $\mu \neq 0$, risk $\to 1$ as $T \to \infty$, the risk of the MLE
- For $\mu = 0$, risk $\nrightarrow 0$, risk of "zero" estimator
- Max risk is bounded

BIC

- For any $\mu \neq 0$, risk $\to 1$ as $T \to \infty$, the risk of the MLE
- For $\mu = 0$, risk $\to 0$, risk of "zero" estimator
- Max risk is unbounded

Lecture #5 – Andrews (1999) Moment Selection Criteria

Lightning Review of GMM

The J-test Statistic Under Correct Specification

The J-test Statistic Under Mis-specification

Andrews (1999; Econometrica)

Generalized Method of Moments (GMM) Estimation

Notation

Let v_t be a $(r \times 1)$ random vector, θ be a $(p \times 1)$ parameter vector, and f be a $(q \times 1)$ vector of real-valued functions.

Popn. Moment Conditions

$$\mathbb{E}\left[f(v_t, \theta_0)\right] = 0$$

Sample Moment Conditions

$$\bar{g}_T(\theta) = \frac{1}{T}\sum_{t=1}^{T} f(v_t, \theta)$$

GMM Estimator

$$\widehat{\theta}_T = \underset{\theta \in \Theta}{\arg\min}\ \bar{g}_T(\theta)' \underset{(q\times q)}{W_T}\ \bar{g}_T(\theta), \quad W_T \to_p W \text{ (psd)}$$

Key Assumptions for GMM I

Stationarity

The sequence $\{v_t : -\infty < t < \infty\}$ is strictly stationary. This implies that *any* moments of v_t are constant over t.

Global Identification

$\mathbb{E}[f(v_t, \theta_0)] = 0$ but $\mathbb{E}[f(v_t, \widetilde{\theta})] \neq 0$ for any $\widetilde{\theta} \neq \theta_0$.

Regularity Conditions for Moment Functions

$f : \mathcal{V} \times \Theta \to \mathbb{R}^q$ satisfies:

(i) f is v_t-almost surely continuous on Θ

(ii) $E[f(v_t, \theta)] < \infty$ exists and is continuous on Θ

Key Assumptions for GMM I

Regularity Conditions for Derivative Matrix

(i) $\nabla_{\theta'} f(v_t, \theta)$ exists and is v_t-almost continuous on Θ

(ii) $E[\nabla_\theta f(v_t, \theta_0)] < \infty$ exists and is continuous in a neighborhood N_ϵ of θ_0

(iii) $\sup_{\theta \in N_\epsilon} \left|\left| T^{-1} \sum_{t=1}^{T} \nabla_\theta f(v_t, \theta) - E[\nabla_\theta f(v_t, \theta)] \right|\right| \xrightarrow{p} 0$

Regularity Conditions for Variance of Moment Conditions

(i) $E[f(v_t, \theta_0) f(v_t, \theta_0)']$ exists and is finite.

(ii) $\lim_{T \to \infty} Var\left[\sqrt{T} \bar{g}_T(\theta_0)\right] = S$ exists and is a finite, positive definite matrix.

Main Results for GMM Estimation

Under the Assumptions Described Above

Consistency: $\widehat{\theta}_T \xrightarrow{p} \theta_0$

Asymptotic Normality: $\sqrt{T}(\widehat{\theta}_T - \theta_0) \xrightarrow{d} \mathcal{N}(0, MSM')$

$$M = (G_0 W G_0)^{-1} G_0' W$$

$$S = \lim_{T\to\infty} Var\left[\sqrt{T}\bar{g}_T(\theta_0)\right]$$

$$G_0 = E[\nabla_{\theta'} f(v_t, \theta_0)]$$

$$W = \text{plim}_{T\to\infty} W_T$$

The J-test Statistic

$$\boxed{J_T = T\ \bar{g}_T(\widehat{\theta}'_T)\ \widehat{S}^{-1}\ \bar{g}_T(\widehat{\theta}_T)}$$

$$\widehat{S} \rightarrow_p S = \lim_{T\rightarrow\infty} Var\left[\sqrt{T}\bar{g}_T(\theta_0)\right]$$

$$\bar{g}_T(\widehat{\theta}_T) = \frac{1}{T}\sum_{t=1}^{T} f(v_t, \widehat{\theta}_T)$$

$$\widehat{\theta}_T = \text{GMM Estimator}$$

Case I: Correct Specification

Suppose that all of the preceding assumptions hold, in particular that the model is correctly specified:

$$\mathbb{E}[f(v_t, \theta_0)] = 0$$

Recall that under the standard assumptions, the GMM estimator is consistent regardless of the choice of $W_T \ldots$

Case I: Taylor Expansion under Correct Specification

$$W_T^{1/2}\sqrt{T}\bar{g}_T(\widehat{\theta}_T) = [I_q - P(\theta_0)]\, W^{1/2}\sqrt{T}\bar{g}_T(\theta_0) + o_p(1)$$

$$\begin{aligned} P(\theta_0) &= F(\theta_0)\left[F(\theta_0)'F(\theta_0)\right]^{-1}F(\theta_0)' \\ F(\theta_0) &= W^{1/2}E[\nabla_\theta f(v_t,\theta_0)] \end{aligned}$$

Over-identification

If $\dim(f) > \dim(\theta_0)$, $W^{1/2}\mathbb{E}[f(v_t,\theta_0)]$ is the linear combn. used in GMM estimation.

Identifying and Over-Identifying Restrictions

$P(\theta_0) \equiv$ **identifying restrictions**;

$I_q - P(\theta_0) \equiv$ **over-identifying restrictions**

J-test Statistic Under Correct Specification

$$W_T^{1/2}\sqrt{T}\bar{g}_T(\widehat{\theta}_T) = [I_q - P(\theta_0)]\, W^{1/2}\sqrt{T}\bar{g}_T(\theta_0) + o_p(1)$$

- CLT for $\sqrt{T}\bar{g}_T(\theta_0)$
- $I_q - P(\theta_0)$ has rank $(q-p)$, since $P(\theta_0)$ has rank p.
- **Singular** normal distribution
- $W_T^{1/2}\sqrt{T}\bar{g}_T(\widehat{\theta}_T) \xrightarrow{d} \mathcal{N}(0, NW^{1/2}SW^{1/2}N')$
- Substituting $\widehat{S}^{-1}$, $J_T \xrightarrow{d} \chi^2_{q-p}$

Case II: Fixed Mis-specification

$$\boxed{\mathbb{E}[f(v_t, \theta)] = \mu(\theta), \quad ||\mu(\theta)|| > 0, \ \forall \theta \in \Theta}$$

N.B.

This can *only* occur in the over-identified case, since we can always solve the population moment conditions in the just-identified case.

Notation

- $\theta^* \equiv$ solution to identifying restrictions ($\widehat{\theta}_T \to_p \theta^*$)
- $\mu^* = \mu(\theta^*) = \text{plim}_{T\to\infty}\bar{g}_T(\widehat{\theta}_T)$

Case II: Fixed Mis-specification

$$\frac{1}{T} J_T = \bar{g}_T(\widehat{\theta}_T)' \widehat{S}^{-1} \bar{g}_T(\widehat{\theta}_T) = \mu_*' W \mu_* + o_p(1)$$

- W positive definite
- since $\mu(\theta) > 0$ for all $\theta \in \Theta$.
- Hence: $\mu_*' W \mu_* > 0$
- Fixed mis-specification $\Rightarrow$ J-test statistic *diverges at rate T*:

$$J_T = T \mu_*' W \mu_* + o_p(T)$$

Summary: Correct Specification vs. Fixed Mis-specification

Correct Specification: $J_T \Rightarrow \chi^2_{q-p} = O_p(1)$

Fixed Mis-specification: $J_T = O_p(T)$

Andrews (1999; Econometrica)

- Family of moment selection criteria (MSC) for GMM
- Aims to **consistently** choose any and all correct MCs and eliminate incorrect MCs
- AIC/BIC: add a **penalty** to maximized log-likelihood
- Andrews MSC: add a **bonus** term to the J-statistic
  - J-stat shows how well MCs "fit"
  - Compares $\widehat{\theta}_T$ estimated using $P(\theta_0)$ to MCs from $I_q - P(\theta_0)$
  - J-stat tends to increase with degree of overidentification even if MCs are correct, since it converges to a χ^2_{q-p}

Andrews (1999) – Notation

$f_{max} \equiv (q \times 1)$ vector of all MCs under consideration

$c \equiv (q \times 1)$ selection vector: zeros and ones indicating which MCs are included

$\mathcal{C} \equiv$ set of all candidates c

$|c| \equiv \#$ of MCs in candidate c

Let $\widehat{\theta}_T(c)$ be the efficient two-step GMM estimator based on the moment conditions $E[f(v_t, \theta, c)] = 0$ and define

$$
\begin{aligned}
V_\theta(c) &= \left[G_0(c) S(c)^{-1} G_0(c)\right]^{-1} \\
G_0(c) &= E[\nabla'_\theta f(v_t, \theta_0; c)] \\
S(c) &= \lim_{T\to\infty} Var\left[\frac{1}{\sqrt{T}} \sum_{t=1}^{T} f(v_t, \theta_0; c)\right] \\
J_T(c) &= T \bar{g}_T\left(\widehat{\theta}_T(c); c\right)' \widehat{S}_T(c)^{-1} \bar{g}_T\left(\widehat{\theta}_T(c); c\right)
\end{aligned}
$$

Identification Condition

- Andrews wants maximal set of correct MCs
  - Consistent, minimum asymptotic variance
- But different θ values could solve $\mathbb{E}[f(v_t, \theta, c)]$ for different c!
- Which θ_0 are we actually trying to be consistent for?

More Notation

- $\mathcal{Z}^0 \equiv$ set of all c for which $\exists\, \theta$ with $\mathbb{E}[f(v_t, \theta, c)] = 0$
- $\mathcal{MZ}^0 \equiv$ subset of $\mathcal{Z}^0$ with **maximal** $|c|$.

Assumption

Andrews assumes that $\mathcal{MZ}^0 = \{c_0\}$, a singleton.

Family of Moment Selection Criteria

- Criteria of the form $MSC(c) = J_T(c) - B(T, |c|)$
- B is a **bonus term** that depends on sample size and # of MCs
- Choose $\widehat{c}_T = \underset{c \in \mathcal{C}}{\arg\min} MSC(c)$
- Implementation Detail: Andrews suggests using a **centered** covariance matrix estimator:

$$\widehat{S}(c) = \frac{1}{T}\sum_{t=1}^{T}\left[f(v_t, \widehat{\theta}_T(c); c) - \bar{g}_T(\widehat{\theta}_T(c); c)\right]\left[f(v_t, \widehat{\theta}_T(c); c) - \bar{g}_T(\widehat{\theta}_T(c); c)\right]'$$

based on the weighting matrix that *would be* efficient if the moment conditions were correctly specified. This remains consistent for $S(c)$ even under fixed mis-specification

Regularity Conditions for the J-test Statistic

(i) If $\mathbb{E}[f(v_t, \theta; c)] = 0$ for a unique $\theta \in \Theta$, then $J_T(c) \xrightarrow{d} \chi^2_{|c|-p}$

(ii) If $\mathbb{E}[f(v_t, \theta; c)] \neq 0$ for a *all* $\theta \in \Theta$ then $T^{-1} J_T(c) \xrightarrow{p} a(c)$, a finite, positive constant that may depend on c.

Regularity Conditions for Bonus Term

The bonus term can be written as $B(|c|, T) = \kappa_T h(|c|)$, where

(i) $h(\cdot)$ is strictly increasing

(ii) $\kappa_T \to \infty$ as $T \to \infty$ and $\kappa_T = o(T)$

Identification Conditions

(i) $\mathcal{MZ}^0 = \{c_0\}$

(ii) $\mathbb{E}[f(v_t, \theta_0; c_0)] = 0$ and $E[f(v_t, \theta; c_0)] \neq 0$ for any $\theta \neq \theta_0$

Consistency of Moment Selection

Theorem

Under the preceding assumptions, $MSC(c)$ is a consistent moment selection criterion, i.e. $\widehat{c}_T \xrightarrow{p} c_0$.

Some Examples

$$\text{GMM-BIC}(c) = J_T(c) - (|c| - p)\log(T)$$

$$\text{GMM-HQ}(c) = J_T(c) - 2.01\,(|c| - p)\log\big(\log(T)\big)$$

$$\text{GMM-AIC}(c) = J_T(c) - 2\,(|c| - p)$$

How do these examples behave?

- GMM-AIC: $\kappa_T = 2$
- GMM-BIC: $\lim_{T\to\infty} \log(T)/T = 0$ ✓
- GMM-HQ: $\lim_{T\to\infty} \log\big(\log(T)\big)/T = 0$ ✓

Proof

Need to show

$$\lim_{T\to\infty} \mathbb{P}\left[\underbrace{\text{MSC}_T(c) - MSE_T(c_0)}_{\Delta_T(c)} > 0\right] = 1 \quad \text{for any } c \neq c_0$$

Defintion of $\text{MSC}_T(c)$

$$\Delta_T(c) = [J_T(c) - J_T(c_0)] + \kappa_T\left[h(|c_0|) - h(|c|)\right]$$

Two Cases

I. Unique θ_1 such that $\mathbb{E}\left[f\left(v_t, \theta_1; c_1\right)\right] = 0 \quad (c_1 \neq c_0)$

II. For all $\theta \in \Theta$ we have $\mathbb{E}\left[f\left(v_t, \theta; c_2\right)\right] \neq 0 \quad (c_2 \neq c_0)$

Case I: $c_1 \neq c_0$ is "correctly specified"

1. Regularity Condition (i) for J-stat. applies to c_0 and c_1

$$J_T(c_1) - J_T(c_0) \to^{\mathrm{d}} \chi^2_{|c_1|-p} - \chi^2_{|c_0|-p} = O_p(1)$$

2. Identification Condition (i) says c_0 is the unique, maximal set of correct moment conditions $\implies |c_0| > |c_1|$
3. Bonus Term Condition (i): h is strictly increasing $\implies h(|c_0|) - h(|c_1|) > 0$
4. Bonus Term Condition (ii): κ_T diverges to infinity $\implies \kappa,_T \left[h(|c_0| - h(|c_1|)\right] \to \infty$
5. Therefore: $\Delta_T(c_1) = O_p(1) + \kappa_T \left[h(|c_0| - h(|c_1|)\right] \to \infty$ ✓

Case II: $c_2 \neq c_0$ is mis-specified

1. Regularity Condition (i) for J-stat. applies to c_0; (ii) applies to c_2

$$\frac{1}{T}\left[J_T(c_2) - J_T(c_0)\right] = \left[a(c_2) + o_p(1)\right] + \left[\frac{1}{T}\chi^2_{|c_0|-p}\right] = a(c_2) + o_p(1)$$

2. Bonus Term Condition (ii): h is strictly increasing. Since $|c_0|$ and $|c_2|$ are finite $\implies$ $[h(|c_0|) - h(|c_1|)]$ is finite
3. Bonus Term Condition (i): $\kappa_T = o(T)$. Combined with prev. step:

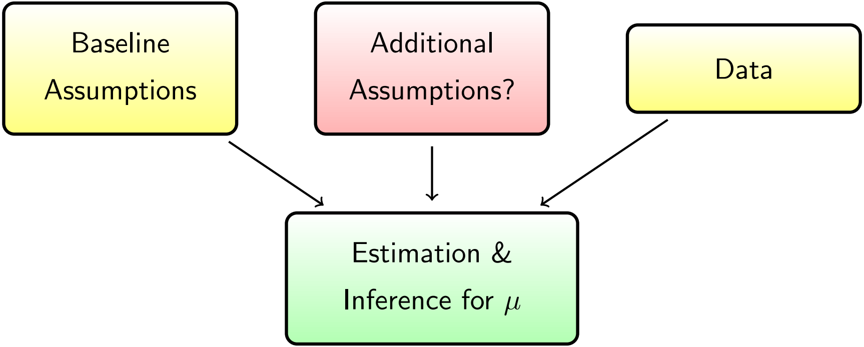
$$\frac{1}{T}\left[\kappa_T \left\{h(|c_0|) - h(|c_2|)\right\}\right] = \frac{1}{T}\left[o(T) \times \text{Constant}\right] = o(1)$$

4. (1 and 3) $\implies$ $\frac{1}{T}\Delta_T(c_2) = a(c_2) + o_p(1) + o(1) \to^p a(c_2) > 0$
5. Therefore $\Delta_T(c_2) \to \infty$ wpa 1 as $T \to \infty$.

Lecture #6 – Focused Moment Selection

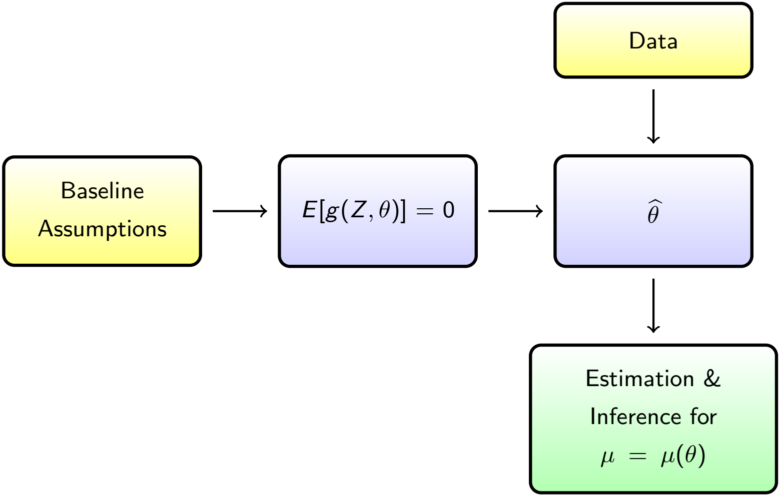
DiTraglia (2016, JoE)

Focused Moment Selection Criterion (FMSC)

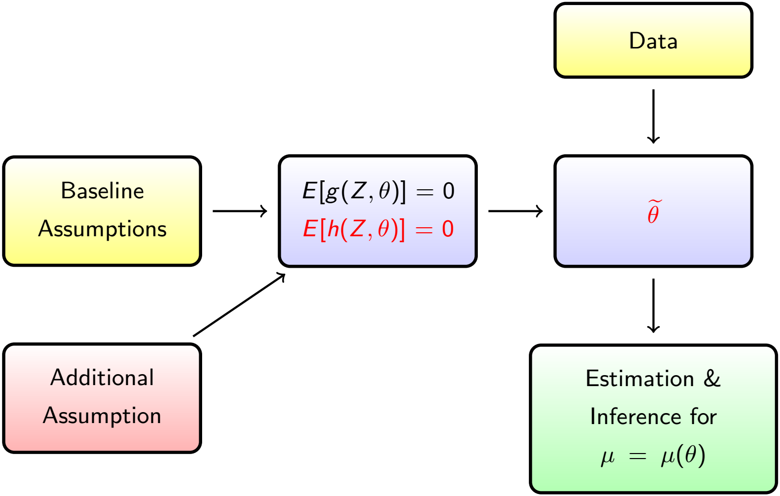


1. Choose False Assumptions on Purpose
2. Focused Choice of Assumptions
3. Local mis-specification
4. Averaging, Inference post-selection

GMM Framework



Adding Moment Conditions



Ordinary versus Two-Stage Least Squares

$$\begin{aligned} y_i &= \beta x_i + \epsilon_i \\ x_i &= \mathbf{z}_i' \boldsymbol{\pi} + v_i \end{aligned}$$

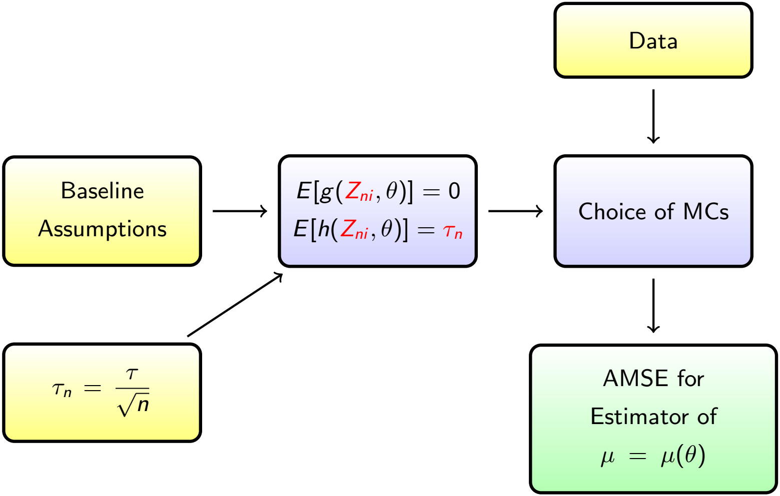
$$\begin{aligned} E[\mathbf{z}_i \epsilon_i] &= 0 \\ E[x_i \epsilon_i] &= ? \end{aligned}$$

Choosing Instrumental Variables

$$
\begin{aligned}
y_i &= \beta x_i + \epsilon_i \\
x_i &= \Pi_1' \mathbf{z}_i^{(1)} + \Pi_2' \mathbf{z}_i^{(2)} + v_i
\end{aligned}
$$

$$
\begin{aligned}
E[\mathbf{z}_i^{(1)} \epsilon_i] &= 0 \\
E[\mathbf{z}_i^{(2)} \epsilon_i] &= ?
\end{aligned}
$$

FMSC Asymptotics – Local Mis-Specification



Local Mis-Specification for OLS versus TSLS

$$\begin{aligned} y_i &= \beta x_i + \epsilon_i \\ x_i &= \mathbf{z}_i' \boldsymbol{\pi} + v_i \end{aligned}$$

$$\begin{aligned} E[\mathbf{z}_i \epsilon_i] &= 0 \\ E[x_i \epsilon_i] &= \tau/\sqrt{n} \end{aligned}$$

Local Mis-Specification for Choosing IVs

$$
\begin{aligned}
y_i &= \beta x_i + \epsilon_i \\
x_i &= \Pi_1' \mathbf{z}_i^{(1)} + \Pi_2' \mathbf{z}_i^{(2)} + v_i
\end{aligned}
$$

$$
\begin{aligned}
E[\mathbf{z}_i^{(1)} \epsilon_i] &= 0 \\
E[\mathbf{z}_i^{(2)} \epsilon_i] &= \tau/\sqrt{n}
\end{aligned}
$$

Local Mis-Specification

Triangular Array $\{Z_{ni} \colon 1 \leq i \leq n, n = 1, 2, \ldots\}$ with

(a) $E[g(Z_{ni}, \theta_0)] = 0$

(b) $E[h(Z_{ni}, \theta_0)] = n^{-1/2}\tau$

(c) $\{f(Z_{ni}, \theta_0) \colon 1 \leq i \leq n, n = 1, 2, \ldots\}$ uniformly integrable

(d) $Z_{ni} \rightarrow_d Z_i$, where the Z_i are identically distributed.

Shorthand: Write Z for Z_i

Candidate GMM Estimator

$$\widehat{\theta}_S = \underset{\theta \in \Theta}{\arg\min} \; [\Xi_S f_n(\theta)]' \, \widetilde{W}_S \; [\Xi_S f_n(\theta)]$$

$$\begin{aligned}
\Xi_S &= \text{Selection Matrix (ones and zeros)} \\
\widetilde{W}_S &= \text{Weight Matrix (p.s.d.)} \\
f_n(\theta) &= \begin{bmatrix} g_n(\theta) \\ h_n(\theta) \end{bmatrix} = \begin{bmatrix} n^{-1} \sum_{i=1}^n g(Z_{ni}, \theta) \\ n^{-1} \sum_{i=1}^n h(Z_{ni}, \theta) \end{bmatrix}
\end{aligned}$$

Notation: Limit Quantities

$$G = E\left[\nabla_\theta\, g(Z, \theta_0)\right], \quad H = E\left[\nabla_\theta\, h(Z, \theta_0)\right], \quad F = \begin{bmatrix} G \\ H \end{bmatrix}$$

$$\Omega = Var\left[f(Z, \theta_0)\right] = \begin{bmatrix} \Omega_{gg} & \Omega_{gh} \\ \Omega_{hg} & \Omega_{hh} \end{bmatrix}$$

$$\widetilde{W}_S \to_p W_S \text{ (p.d.)}$$

Local Mis-Specification + Standard Regularity Conditions

Every candidate estimator is consistent for θ_0 and

$$\sqrt{n}(\widehat{\theta}_S - \theta_0) \to_d -K_S \Xi_S \left(\begin{bmatrix} M_g \\ M_h \end{bmatrix} + \begin{bmatrix} 0 \\ \tau \end{bmatrix} \right)$$

$$\begin{aligned} K_S &= [F_S' W_S F_S]^{-1} F_S' W_S \\ M &= (M_g', M_h')' \\ M &\sim N(0, \Omega) \end{aligned}$$

Scalar Target Parameter μ

$$\begin{aligned} \mu &= \mu(\theta) && \text{Z-a.s. continuous function} \\ \mu_0 &= \mu(\theta_0) && \text{true value} \\ \widehat{\mu}_S &= \mu(\widehat{\theta}_S) && \text{estimator} \end{aligned}$$

Delta Method

$$\sqrt{n}\left(\widehat{\mu}_S - \mu_0\right) \rightarrow_d -\nabla_\theta \mu(\theta_0)' K_S \Xi_S \left(M + \begin{bmatrix} 0 \\ \tau \end{bmatrix}\right)$$

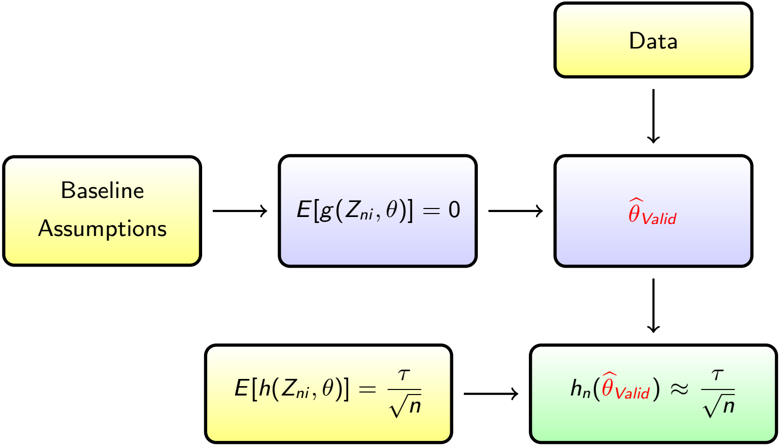
FMSC: Estimate AMSE($\widehat{\mu}_S$) and minimize over S

$$\text{AMSE}\left(\widehat{\mu}_S\right) = \nabla_\theta \mu(\theta_0)' K_S \Xi_S \left\{ \begin{bmatrix} 0 & 0 \\ 0 & \tau\tau' \end{bmatrix} + \Omega \right\} \Xi_S' K_S' \nabla_\theta \mu(\theta_0)$$

Estimating the unknowns

No consistent estimator of τ exists! (But everything else is easy)

A Plug-in Estimator of τ



An Asymptotically Unbiased Estimator of $\tau\tau'$

$$\sqrt{n}h_n(\widehat{\theta}_v) = \widehat{\tau} \to_d (\Psi M + \tau) \sim N_q(\tau, \Psi\Omega\Psi')$$

$$\Psi = \left[\begin{array}{cc} -HK_v & \mathbf{I}_q \end{array} \right]$$

$\widehat{\tau}\widehat{\tau}' - \widehat{\Psi}\widehat{\Omega}\widehat{\Psi}$ is an asymptotically unbiased estimator of $\tau\tau'$.

FMSC: Asymptotically Unbiased Estimator of AMSE

$$\text{FMSC}_n(S) = \nabla_\theta \mu(\widehat{\theta})' \widehat{K}_S \Xi_S \left\{ \begin{bmatrix} 0 & 0 \\ 0 & \widehat{B} \end{bmatrix} + \widehat{\Omega} \right\} \Xi_S' \widehat{K}_S' \nabla_\theta \mu(\widehat{\theta})$$

$$\widehat{B} = \widehat{\tau}\widehat{\tau}' - \widehat{\Psi}\widehat{\Omega}\widehat{\Psi}'$$

Choose S to minimize $\text{FMSC}_n(S)$ over the set of candidates $\mathscr{S}$.

A (Very) Special Case of the FMSC

Under homoskedasticity, FMSC selection in the OLS versus TSLS example is *identical* to a Durbin-Hausman-Wu test with $\alpha \approx 0.16$

$$\widehat{\tau} = n^{-1/2}\mathbf{x}'(\mathbf{y} - \mathbf{x}\widetilde{\beta}_{TSLS})$$

OLS gets benefit of the doubt, but not as much as $\alpha = 0.05,\ 0.1$

Limit Distribution of FMSC

$FMSC_n(S) \rightarrow_d FMSC_S$, where

$$
\begin{aligned}
\text{FMSC}_S &= \nabla_\theta \mu(\theta_0)' K_S \Xi_S \left\{ \left[\begin{array}{cc} 0 & 0 \\ 0 & B \end{array} \right] + \Omega \right\} \Xi_S' K_S' \nabla_\theta \mu(\theta_0) \\
B &= (\Psi M + \tau)(\Psi M + \tau)' - \Psi \Omega \Psi'
\end{aligned}
$$

Conservative criterion: random even in the limit.

Moment Average Estimators

$$\widehat{\mu} = \sum_{S \in \mathscr{S}} \widehat{\omega}_S \widehat{\mu}_S$$

Additional Notation

- $\widehat{\mu}$ Moment-average Estimator
- $\widehat{\mu}_S$ Estimator of target parameter under moment set S
- $\widehat{\omega}_S$ Data-dependent weight function
- $\mathscr{S}$ Collection of moment sets under consideration

Examples of Moment-Averaging Weights

Post-Moment Selection Weights

$\widehat{\omega}_S = \mathbf{1}\left\{\text{MSC}_n(S) = \min_{S' \in \mathscr{S}} \text{MSC}_n(S')\right\}$

Exponential Weights

$$\widehat{\omega}_S = \exp\left\{-\frac{\kappa}{2}\text{MSC}(S)\right\} \Big/ \sum_{S' \in \mathscr{S}} \exp\left\{-\frac{\kappa}{2}\text{MSC}(S')\right\}$$

Minimum-AMSE Weights...

Minimum AMSE-Averaging Estimator: OLS vs. TSLS

$$\widetilde{\beta}(\omega) = \omega \widehat{\beta}_{OLS} + (1-\omega)\widetilde{\beta}_{TSLS}$$

Under homoskedasticity:

$$\omega^* = \left[1 + \frac{\text{ABIAS(OLS)}^2}{\text{AVAR(TSLS)} - \text{AVAR(OLS)}}\right]^{-1}$$

Estimate by:

$$\widehat{\omega}^* = \left[1 + \frac{\max\left\{0,\ \left(\widehat{\tau}^2 - \widehat{\sigma}_\epsilon^2 \widehat{\sigma}_x^2 \left(\widehat{\sigma}_x^2/\widehat{\gamma}^2 - 1\right)\right) / \ \widehat{\sigma}_x^4\right\}}{\widehat{\sigma}_\epsilon^2(1/\widehat{\gamma}^2 - 1/\widehat{\sigma}_x^2)}\right]^{-1}$$

Where $\widehat{\gamma}^2 = n^{-1}\mathbf{x}'Z(Z'Z)^{-1}Z'\mathbf{x}$

Limit Distribution of Moment-Average Estimators

$$\widehat{\mu} = \sum_{S \in \mathscr{S}} \widehat{\omega}_S \widehat{\mu}_S$$

(i) $\sum_{S \in \mathscr{S}} \widehat{\omega}_S = 1$ a.s.

(ii) $\widehat{\omega}(S) \rightarrow_d \varphi_S(\tau, M)$ a.s.-continuous function of τ, M and consistently-estimable constants only

$$\sqrt{n}\left(\widehat{\mu} - \mu_0\right) \rightarrow_d \Lambda(\tau)$$

$$\Lambda(\tau) = -\nabla_\theta \mu(\theta_0)' \left[\sum_{S \in \mathscr{S}} \varphi_S(\tau, M) K_S \Xi_S\right] \left(M + \left[\begin{array}{c} 0 \\ \tau \end{array}\right]\right)$$

Simulating from the Limit Experiment

Suppose τ Known, Consistent Estimators of Everything Else

1. `for` $j \in \{1, 2, \ldots, J\}$
   (i) $M_j \overset{iid}{\sim} N_{p+q}\left(0, \widehat{\Omega}\right)$
   (ii) $\Lambda_j(\tau) = -\nabla_\theta \mu(\widehat{\theta})' \left[\sum_{S \in \mathscr{S}} \widehat{\varphi}_S(M_j + \tau)\widehat{K}_S \Xi_S\right](M_j + \tau)$
2. Using $\{\Lambda_j(\tau)\}_{j=1}^J$ calculate $\widehat{a}(\tau)$, $\widehat{b}(\tau)$ such that
$$P\left[\widehat{a}(\tau) \leq \Lambda(\tau) \leq \widehat{b}(\tau)\right] = 1 - \alpha$$
3. $P\left[\widehat{\mu} - \widehat{b}(\tau)/\sqrt{n} \leq \mu_0 \leq \widehat{\mu} - \widehat{a}(\tau)/\sqrt{n}\right] \approx 1 - \alpha$

Two-step Procedure for Conservative Intervals

1. Construct $1-\delta$ confidence region $\mathscr{T}(\widehat{\tau}, \delta)$ for τ
2. For each $\tau^* \in \mathscr{T}(\widehat{\tau}, \delta)$ calculate $1-\alpha$ confidence interval $\left[\widehat{a}(\tau^*), \widehat{b}(\tau^*)\right]$ for $\Lambda(\tau^*)$ as descibed on previous slide.
3. Take the lower and upper bound over the resulting intervals: $\widehat{a}_{min}(\widehat{\tau}) = \min_{\tau^* \in \mathscr{T}} \widehat{a}(\tau^*), \quad \widehat{b}_{max}(\widehat{\tau^*}) = \max_{\tau^* \in \mathscr{T}} \widehat{b}(\tau)$
4. The interval

$$\text{CI}_{sim} = \left[\widehat{\mu} - \frac{\widehat{b}_{max}(\widehat{\tau})}{\sqrt{n}}, \quad \widehat{\mu} - \frac{\widehat{a}_{min}(\widehat{\tau})}{\sqrt{n}}\right]$$

has asymptotic coverage of at least $1-(\alpha+\delta)$

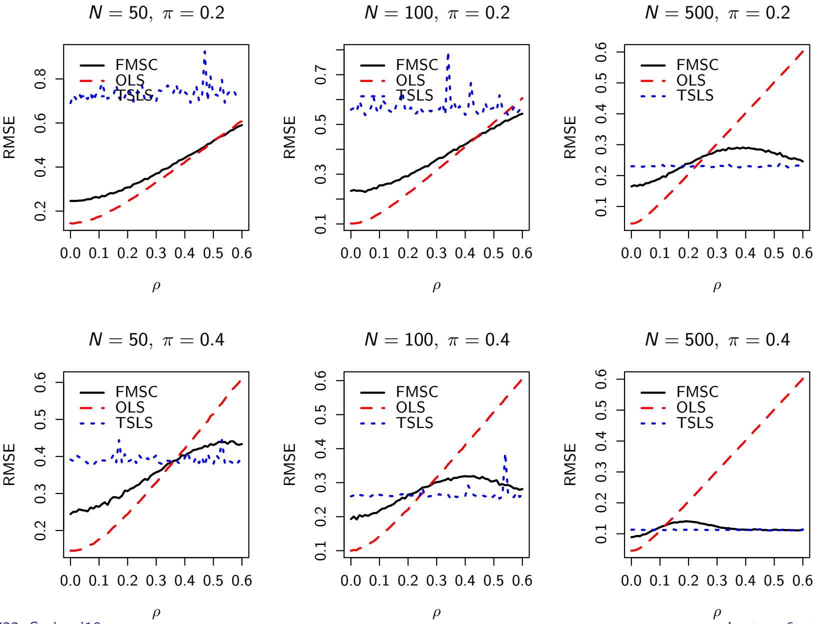
OLS versus TSLS Simulation

$$
\begin{aligned}
y_i &= 0.5x_i + \epsilon_i \\
x_i &= \pi(z_{1i} + z_{2i} + z_{3i}) + v_i
\end{aligned}
$$

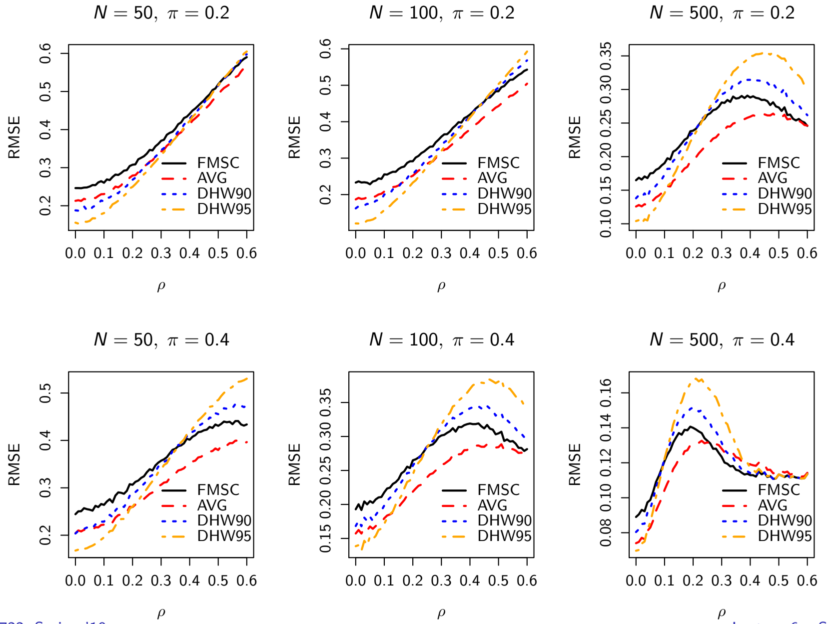
$$(\epsilon_i, v_i, z_{1i}, z_{2i}, z_{3i}) \sim \text{ iid } N(0, \mathcal{S})$$

$$
\mathcal{S} = \begin{bmatrix}
1 & \rho & 0 & 0 & 0 \\
\rho & 1-\pi^2 & 0 & 0 & 0 \\
0 & 0 & 1/3 & 0 & 0 \\
0 & 0 & 0 & 1/3 & 0 \\
0 & 0 & 0 & 0 & 1/3
\end{bmatrix}
$$

$$Var(x) = 1, \qquad \rho = Cor(x, \epsilon), \qquad \pi^2 = \text{First-Stage } R^2$$



$N = 50,\ \pi = 0.2$
$N = 100,\ \pi = 0.2$
$N = 500,\ \pi = 0.2$
$N = 50,\ \pi = 0.4$
$N = 100,\ \pi = 0.4$
$N = 500,\ \pi = 0.4$
FMSC
OLS
TSLS
RMSE
ρ
0.0 0.1 0.2 0.3 0.4 0.5 0.6



$N = 50,\ \pi = 0.2$
$N = 100,\ \pi = 0.2$
$N = 500,\ \pi = 0.2$
$N = 50,\ \pi = 0.4$
$N = 100,\ \pi = 0.4$
$N = 500,\ \pi = 0.4$
RMSE
ρ
FMSC
AVG
DHW90
DHW95
0.0 0.1 0.2 0.3 0.4 0.5 0.6

Choosing Instrumental Variables Simulation

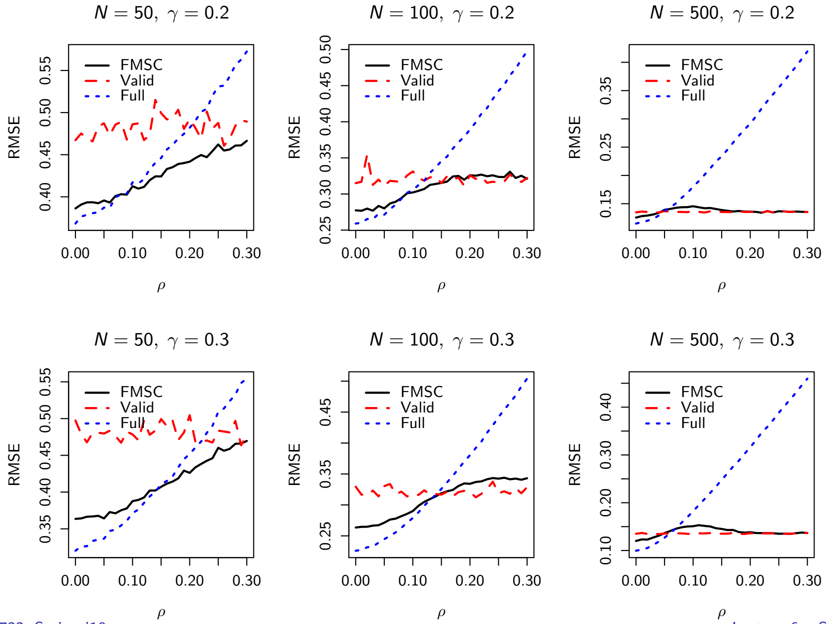
$$\begin{aligned} y_i &= 0.5x_i + \epsilon_i \\ x_i &= (z_{1i} + z_{2i} + z_{3i})/3 + \gamma w_i + v_i \end{aligned}$$

$$(\epsilon_i, v_i, w_i, z_{i1}, z_{2i}, z_{3i})' \sim \text{ iid } N(0, \mathcal{V})$$

$$\mathcal{V} = \begin{bmatrix} 1 & (0.5 - \gamma\rho) & \rho & 0 & 0 & 0 \\ (0.5 - \gamma\rho) & (8/9 - \gamma^2) & 0 & 0 & 0 & 0 \\ \rho & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/3 \end{bmatrix}$$

$$\gamma = Cor(x, w), \quad \rho = Cor(w, \epsilon), \quad \text{First-Stage } R^2 = 1/9 + \gamma^2$$

$$Var(x) = 1, \quad Cor(x, \epsilon) = 0.5$$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$N = 500,\ \gamma = 0.2$
$N = 50,\ \gamma = 0.3$
$N = 100,\ \gamma = 0.3$
$N = 500,\ \gamma = 0.3$
RMSE
ρ
FMSC
Valid
Full
0.00
0.10
0.20
0.30

Alternative Moment Selection Procedures

Downward J-test

Use Full instrument set unless J-test rejects.

Andrews (1999) – GMM Moment Selection Criteria

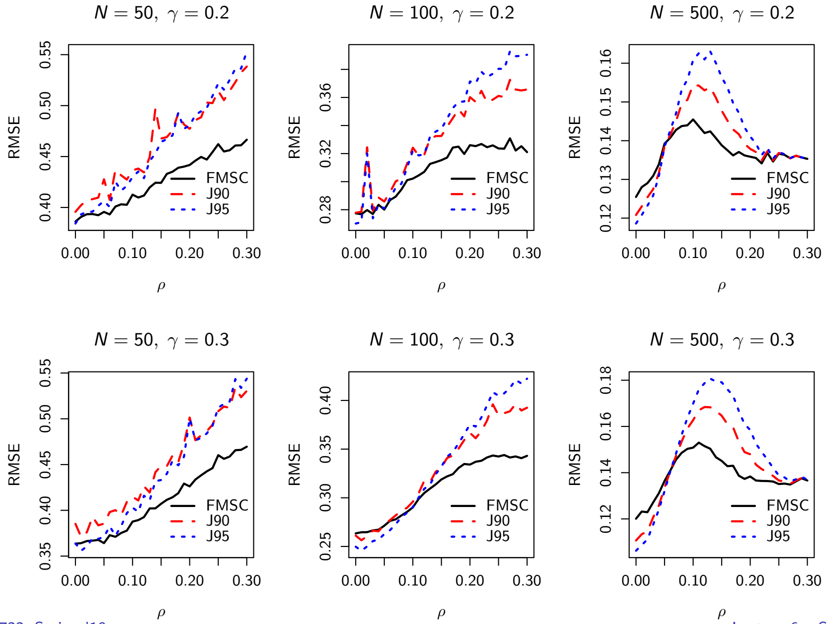
$\text{GMM-MSC}(S) = J_n(S) - \text{Bonus}$

Hall & Peixe (2003) – Canonical Correlations Info. Criterion

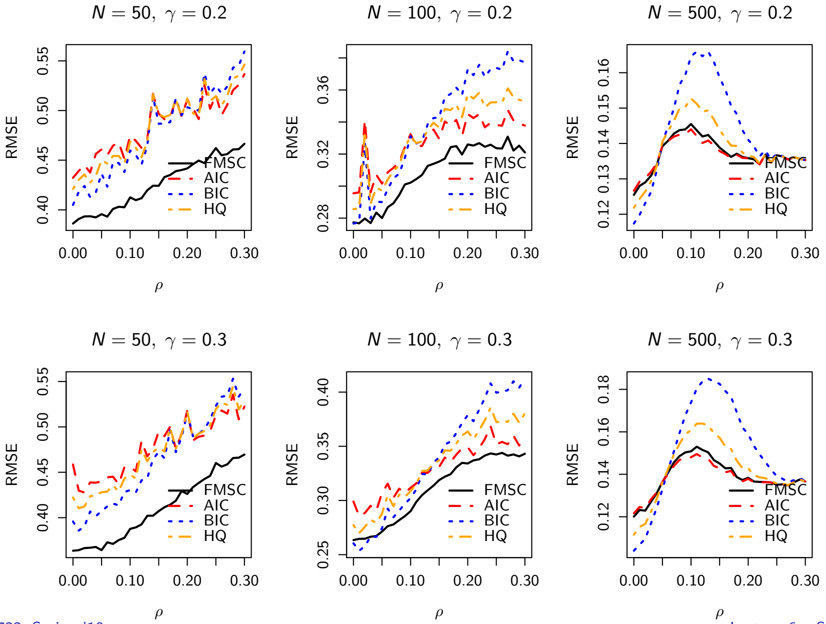
$\text{CCIC}(S) = n \log \left[1 - R_n^2(S)\right] + \textit{Penalty}$

Penalty/Bonus Terms

Analogies to AIC, BIC, and Hannan-Quinn



$N = 50,\ \gamma = 0.2$
$N = 100,\ \gamma = 0.2$
$N = 500,\ \gamma = 0.2$
$N = 50,\ \gamma = 0.3$
$N = 100,\ \gamma = 0.3$
$N = 500,\ \gamma = 0.3$
RMSE
ρ
FMSC
J90
J95
0.00
0.10
0.20
0.30



$N = 50,\ \gamma = 0.2$
$N = 100,\ \gamma = 0.2$
$N = 500,\ \gamma = 0.2$
$N = 50,\ \gamma = 0.3$
$N = 100,\ \gamma = 0.3$
$N = 500,\ \gamma = 0.3$
RMSE
ρ
FMSC
AIC
BIC
HQ

Empirical Example: Geography or Institutions?

Institutions Rule

Acemoglu et al. (2001), Rodrik et al. (2004), Easterly & Levine (2003) – zero or negligible effects of "tropics, germs, and crops" in income per capita, controlling for institutions.

Institutions *Don't* Rule

Sachs (2003) – Large negative direct effect of malaria transmission on income.

Carstensen & Gundlach (2006)

How robust is Sachs's result?

Carstensen & Gundlach (2006)

Both Regressors Endogenous

$$\ln GDPC_i = \beta_1 + \beta_2 \cdot INSTITUTIONS_i + \beta_3 \cdot MALARIA_i + \epsilon_i$$

Robustness

- Various measures of *INSTITUTIONS*, *MALARIA*
- Various instrument sets
- β_3 remains large, negative and significant.

2SLS for All Results That Follow

Expand on Instrument Selection Exercise

FMSC and Corrected Confidence Intervals

1. FMSC – which instruments to estimate effect of malaria?
2. Correct CIs for Instrument Selection – effect of malaria still negative and significant?

Measures of *INSTITUTIONS* and *MALARIA*

- *rule* – Average governance indicator (Kaufmann, Kray and Mastruzzi; 2004)
- *malfal* – Proportion of population at risk of malaria transmission in 1994 (Sachs, 2001)

Instrument Sets

Baseline Instruments – Assumed Valid

- ln*mort* – Log settler mortality (per 1000), early 19th century
- *maleco* – Index of stability of malaria transmission

Further Instrument Blocks

Climate	*frost*, *humid*, *latitude*
Europe	*eurfrac*, *engfrac*
Openness	*coast*, *trade*

	$\mu = \textit{malfal}$			$\mu = \textit{rule}$		
	FMSC	posFMSC	$\widehat{\mu}$	FMSC	posFMSC	$\widehat{\mu}$
(1) Valid	3.0	3.0	-1.0	1.3	1.3	0.9
(2) Climate	3.1	3.1	-0.9	1.0	1.0	1.0
(3) Open	2.3	2.4	-1.1	1.2	1.2	0.8
(4) Eur	1.8	2.2	-1.1	0.5	0.7	0.9
(5) Climate, Eur	0.9	2.0	-1.0	0.3	0.6	0.9
(6) Climate, Open	1.9	2.3	-1.0	0.5	0.8	0.9
(7) Open, Eur	1.6	1.8	-1.2	0.8	0.8	0.8
(8) Full	0.5	1.7	-1.1	0.2	0.6	0.8
$>90\%$ CI FMSC		$(-1.6, -0.6)$			$(0.5, 1.2)$	
$>90\%$ CI posFMSC		$(-1.6, -0.6)$			$(0.6, 1.3)$	

Lecture #7 – High-Dimensional Regression I

QR Decomposition

Singular Value Decomposition

Ridge Regression

Comparing OLS and Ridge

QR Decomposition

Result

Any $n \times k$ matrix A with full column rank can be decomposed as $A = QR$, where R is an $k \times k$ upper triangular matrix and Q is an $n \times k$ matrix with orthonormal columns.

Notes

- Columns of A are *orthogonalized* in Q via Gram-Schmidt.
- Since Q has orthogonal columns, $Q'Q = I_k$.
- It is *not* in general true that $QQ' = I$.
- If A is square, then $Q^{-1} = Q'$.

Different Conventions for the QR Decomposition

Thin aka Economical QR

Q is an $n \times k$ with orthonormal columns (`qr_econ` in Armadillo).

Thick QR

Q is an $n \times n$ *orthogonal* matrix.

Relationship between Thick and Thin

Let $A = QR$ be the "thick" QR and $A = Q_1 R_1$ be the "thin" QR:

$$A = QR = Q \begin{bmatrix} R_1 \\ 0 \end{bmatrix} = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \begin{bmatrix} R_1 \\ 0 \end{bmatrix} = Q_1 R_1$$

My preferred convention is the thin QR...

Least Squares via QR Decomposition

Let $X = QR$

$$
\begin{aligned}
\widehat{\beta} &= (X'X)^{-1}X'y = \left[(QR)'(QR)\right]^{-1}(QR)'y \\
&= \left[R'Q'QR\right]^{-1}R'Q'y = (R'R)^{-1}R'Qy \\
&= R^{-1}(R')^{-1}R'Q'y = R^{-1}Q'y
\end{aligned}
$$

In other words, $\widehat{\beta}$ solves $R\beta = Q'y$.

Why Bother?

Much easier and faster to solve $R\beta = Q'y$ than the normal equations $(X'X)\beta = X'y$ since R is upper triangular.

Back-Substitution to Solve $R\beta = Q'y$

The product $Q'y$ is a vector, call it v, so the system is simply

$$\begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1,n-1} & r_{1k} \\ 0 & r_{22} & r_{23} & \cdots & r_{2,n-1} & r_{2k} \\ 0 & 0 & r_{33} & \cdots & r_{3,n-1} & r_{3k} \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & r_{k-1,k-1} & r_{k-1,k} \\ 0 & 0 & \cdots & 0 & 0 & r_k \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \\ \beta_{k-1} \\ \beta_k \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_{k-1} \\ v_k \end{bmatrix}$$

$\beta_k = v_k / r_k \Rightarrow$ substitute this into $\beta_{k-1} r_{k-1,k-1} + \beta_k r_{k-1,k} = v_{k-1}$ to solve for β_{k-1}, and so on.

Calculating the Least Squares Variance Matrix $\sigma^2(X'X)^{-1}$

- Since $X = QR$, $(X'X)^{-1} = R^{-1}(R^{-1})'$
- Easy to invert R: just apply repeated back-substitution:
  - Let $A = R^{-1}$ and $\mathbf{a}_j$ be the jth column of A.
  - Let $\mathbf{e}_j$ be the jth standard basis vector.
  - Inverting R is equivalent to solving $R\mathbf{a}_1 = \mathbf{e}_1$, followed by $R\mathbf{a}_2 = \mathbf{e}_2$, ..., $R\mathbf{a}_k = \mathbf{e}_k$.
- If you enclose a matrix in `trimatu()` or `trimatl()`, and request the inverse $\Rightarrow$ Armadillo will carry out backward or forward substitution, respectively.

QR Decomposition for Orthogonal Projections

Let X have full column rank and define $P_X = X(X'X)^{-1}X'$

$$P_X = QR(R'R)^{-1}R'Q' = QRR^{-1}(R')^{-1}R'Q' = QQ'$$

It is *not* in general true that $QQ' = I$ even though $Q'Q = I$ since Q need not be square in the economical QR decomposition.

The Singular Value Decomposition (SVD)

Any $m \times n$ matrix A of arbitrary rank r can be written

$$A = UDV' = (\text{orthogonal})(\text{diagonal})(\text{orthogonal})$$

- $U = m \times m$ orthog. matrix whose cols contain e-vectors of AA'
- $V = n \times n$ orthog. matrix whose cols contain e-vectors of $A'A$
- $D = m \times n$ matrix whose first r main diagonal elements are the *singular values* $d_1, \ldots, d_r$. All other elements are zero.
- The singular values $d_1, \ldots, d_r$ are the square roots of the non-zero eigenvalues of $A'A$ and AA'.
- (E-values of $A'A$ and AA' could be zero but not negative)

SVD for Symmetric Matrices

If A is **symmetric** then $A = Q\Lambda Q'$ where Λ is a diagonal matrix containing the e-values of A and Q is an orthonormal matrix whose columns are the corresponding e-vectors. Accordingly:

$$AA' = (Q\Lambda Q')(Q\Lambda Q')' = Q\Lambda Q' Q\Lambda Q' = Q\Lambda^2 Q'$$

and similarly

$$A'A = (Q\Lambda Q')'(Q\Lambda Q') = Q\Lambda Q' Q\Lambda Q' = Q\Lambda^2 Q'$$

using the fact that Q is orthogonal and Λ diagonal. Thus, when A is symmetric the SVD reduces to $U = V = Q$ and $D = \sqrt{\Lambda^2}$ so that *negative* eigenvalues become *positive* singular values.

The Economical SVD

- Number of singular values is $r = \text{Rank}(A) \leq \max\{m, n\}$
- Some cols of U or V multiplied by zeros in D
- Economical SVD: only keep columns in U and V that are multiplied by non-zeros in D (Armadillo: `svd_econ`)
- Summation form: $A = \sum_{i=1}^{r} d_i \mathbf{u}_i \mathbf{v}_i'$ where $d_1 \leq d_2 \leq \cdots \leq d_r$
- Matrix form: $\underset{(n \times p)}{A} = \underset{(n \times r)}{U} \underset{(r \times r)}{D} \underset{(r \times p)}{V'}$

In the economical SVD, U and V may no longer be square, so they are not orthogonal matrices but their *columns* are still orthonormal.

Ridge Regression – OLS with an L_2 Penalty

$$\widehat{\beta}_{Ridge} = \arg\min_{\beta} \, (\mathbf{y} - X\beta)'(\mathbf{y} - X\beta) + \lambda\beta'\beta$$

- Add a penalty for large coefficients
- $\lambda =$ non-negative constant we choose: strength of penalty
- X and $\mathbf{y}$ assumed to be de-meaned (don't penalize intercept)
- Unlike OLS, Ridge Regression is not scale invariant
  - In OLS if we replace $\mathbf{x}_1$ with $c\mathbf{x}_1$ then β_1 becomes β_1/c.
  - The same is not true for ridge regression!
  - Typical to standardize X before carrying out ridge regression

Alternative Formulation of Ridge Regression Problem

$$\widehat{\beta}_{Ridge} = \underset{\beta}{\arg\min}\; (\mathbf{y} - X\beta)'(\mathbf{y} - X\beta) \quad \text{subject to} \quad \beta'\beta \leq t$$

- Ridge Regression is like least squares "on a budget."
- Make one coefficient larger $\Rightarrow$ must make another one smaller.
- One-to-one mapping from t to λ (data-dependent)

Ridge as Bayesian Linear Regression

If we ignore the intercept, which is unpenalized, Ridge Regression gives the posterior mode from the Bayesian regression model:

$$\begin{aligned} y|X, \beta, \sigma^2 &\sim N(X\beta, \sigma^2 I_n) \\ \beta &\sim N(\mathbf{0}, \tau^2 I_p) \end{aligned}$$

where σ^2 is assumed known and $\lambda = \sigma^2/\tau^2$. (In this example, the posterior is normal so the mode equals the mean)

Explicit Solution to the Ridge Regression Problem

Objective Function:

$$\begin{aligned} Q(\beta) &= (\mathbf{y} - X\beta)'(\mathbf{y} - X\beta) + \lambda\beta'\beta \\ &= \mathbf{y}'\mathbf{y} - \beta' X\mathbf{y} - \mathbf{y}'X\beta + \beta'X'X\beta + \lambda\beta' I_p \beta \\ &= \mathbf{y}'\mathbf{y} - 2\mathbf{y}'X\beta + \beta'(X'X + \lambda I_p)\beta \end{aligned}$$

Recall the following facts about matrix differentiation

$$\partial(\mathbf{a}'\mathbf{x})/\partial\mathbf{x} = \mathbf{a}, \quad \partial(\mathbf{x}'A\mathbf{x})/\partial\mathbf{x} = (A + A')\mathbf{x}$$

Thus, since $(X'X + \lambda I_p)$ is symmetric,

$$\frac{\partial}{\partial\beta} Q(\beta) = -2X'\mathbf{y} + 2(X'X + \lambda I_p)\beta$$

Explicit Solution to the Ridge Regression Problem

Previous Slide:

$$\frac{\partial}{\partial\beta} Q(\beta) = -2X'\mathbf{y} + 2(X'X + \lambda I_p)\beta$$

First order condition:

$$X'\mathbf{y} = (X'X + \lambda I_p)\beta$$

Hence,

$$\widehat{\beta}_{Ridge} = (X'X + \lambda I_p)^{-1} X'\mathbf{y}$$

But is $(X'X + \lambda I_p)$ guaranteed to be invertible?

Ridge Regresion via OLS with "Dummy Observations"

Ridge regression solution is identical to

$$\underset{\beta}{\arg\min}\left(\widetilde{\mathbf{y}}-\widetilde{X}\beta\right)'\left(\widetilde{\mathbf{y}}-\widetilde{X}\beta\right)$$

where

$$\widetilde{\mathbf{y}}=\left[\begin{array}{c}\mathbf{y}\\ \mathbf{0}_p\end{array}\right],\qquad \widetilde{X}=\left[\begin{array}{c}X\\ \sqrt{\lambda}I_p\end{array}\right]$$

since:

$$\begin{aligned}\left(\widetilde{\mathbf{y}}-\widetilde{X}\beta\right)'\left(\widetilde{\mathbf{y}}-\widetilde{X}\beta\right) &= \left[\begin{array}{cc}(\mathbf{y}-X\beta)' & (-\sqrt{\lambda}\beta)'\end{array}\right]\left[\begin{array}{c}(\mathbf{y}-X\beta)\\ -\sqrt{\lambda}\beta\end{array}\right]\\ &= (\mathbf{y}-X\beta)'(\mathbf{y}-X\beta)+\lambda\beta'\beta\end{aligned}$$

Ridge Regression Solution is Always Unique

Ridge solution is always unique, even if there are more regressors than observations! This follows from the preceding slide:

$$\widehat{\beta}_{Ridge} = \arg\min_{\beta} \left(\widetilde{\mathbf{y}} - \widetilde{X}\beta\right)' \left(\widetilde{\mathbf{y}} - \widetilde{X}\beta\right)$$

$$\widetilde{\mathbf{y}} = \begin{bmatrix} \mathbf{y} \\ \mathbf{0}_p \end{bmatrix}, \; \widetilde{X} = \begin{bmatrix} X \\ \sqrt{\lambda} I_p \end{bmatrix}$$

Columns of $\sqrt{\lambda} I_p$ are linearly independent, so columns of $\widetilde{X}$ are also linearly independent, regardless of whether the same holds for the columns of X.

Efficient Calculations for Ridge Regression

QR Decomposition

Write Ridge as OLS with "dummy observations" with $\widetilde{X} = QR$ so

$$\widehat{\beta}_{Ridge} = (\widetilde{X}'\widetilde{X})^{-1}\widetilde{X}'\widetilde{\mathbf{y}} = R^{-1}Q'\widetilde{\mathbf{y}}$$

which we can obtain by back-solving the system $R\widehat{\beta}_{Ridge} = Q'\widetilde{\mathbf{y}}$.

Singular Value Decomposition

If $p \gg n$, it's much faster to use the SVD rather than the QR decomposition because the rank of X will be n. For implementation details, see Murphy (2012; Section 7.5.2).

Comparing Ridge and OLS

Assumption

Centered data matrix $\underset{(n\times p)}{X}$ with rank p so OLS estimator is unique.

Economical SVD

- $\underset{(n\times p)}{X} = \underset{(n\times p)}{U}\underset{(p\times p)}{D}\underset{(p\times p)}{V'}$ with $U'U = V'V = I_p$, D diagonal
- Hence: $X'X = (UDV')'(UDV') = VDU'UDV' = VD^2V'$
- Since V is square it is an orthogonal matrix: $VV' = I_p$

Comparing Ridge and OLS – The "Hat Matrix"

Using $X = UDV'$ and the fact that V is orthogonal,

$$
\begin{aligned}
H(\lambda) &= X\left(X'X + \lambda I_p\right)^{-1} X' = UDV'\left(VD^2V + \lambda VV'\right)^{-1} VDU' \\
&= UDV'\left(VD^2V' + \lambda VV'\right)^{-1} VDU' \\
&= UDV'\left[V(D^2 + \lambda I_p)V'\right]^{-1} VDU' \\
&= UDV'\left(V'\right)^{-1}\left(D^2 + \lambda I_p\right)^{-1}(V)^{-1} VDU' \\
&= UDV'V\left(D^2 + \lambda I_p\right)^{-1} V'VDU' \\
&= UD\left(D^2 + \lambda I_p\right)^{-1} DU'
\end{aligned}
$$

Model Complexity of Ridge Versus OLS

OLS Case

Number of free parameters equals number of parameters p.

Ridge is more complicated

Even though there are p parameters they are constrained!

Idea: use trace of $H(\lambda)$

$$\text{df}(\lambda) = \text{tr}\left\{H(\lambda)\right\} = \text{tr}\left\{X(X'X + \lambda I_p)^{-1}X'\right\}$$

Why? Works for OLS: $\lambda = 0$

$$\text{df}(0) = \text{tr}\left\{H(0)\right\} = \text{tr}\left\{X(X'X)^{-1}X'\right\} = p$$

Effective Degrees of Freedom for Ridge Regression

Using cyclic permutation property of trace:

$$
\begin{aligned}
\mathrm{df}(\lambda) &= \mathrm{tr}\left\{H(\lambda)\right\} = \mathrm{tr}\left\{X(X'X+\lambda I_p)^{-1}X'\right\} \\
&= \mathrm{tr}\left\{UD\left(D^2+\lambda I_p\right)^{-1}DU'\right\} \\
&= \mathrm{tr}\left\{DU'UD\left(D^2+\lambda I_p\right)^{-1}\right\} \\
&= \mathrm{tr}\left\{D^2\left(D^2+\lambda I_p\right)^{-1}\right\} \\
&= \sum_{j=1}^{p}\frac{d_j^2}{d_j^2+\lambda}
\end{aligned}
$$

- $\mathrm{df}(\lambda) \to 0$ as $\lambda \to \infty$
- $\mathrm{df}(\lambda) = p$ when $\lambda = 0$
- $\mathrm{df}(\lambda) < p$ when $\lambda > 0$

Comparing the MSE of OLS and Ridge

Assumptions

$y = X\beta + \varepsilon$, Fixed X, iid data, homoskedasticity

OLS Estimator: $\widehat{\beta}$

$$\widehat{\beta} = (X'X)^{-1}X'y \implies \text{Bias}(\widehat{\beta}) = 0 \quad \text{Var}(\widehat{\beta}) = \sigma(X'X)^{-1}$$

Ridge Estimator: $\widetilde{\beta}_\lambda$

$$\widehat{\beta}_\lambda = (X'X + \lambda I)^{-1}X'y \implies \text{Bias}(\widetilde{\beta}_\lambda) =? \quad \text{Var}(\widetilde{\beta}_\lambda) =?$$

Calculating The Bias of Ridge Regression

X fixed (or condition or X)

$$\begin{aligned}
\text{Bias}(\widetilde{\beta}_\lambda) &= \mathbb{E}\left[(X'X + \lambda I)^{-1}X'(X\beta + \varepsilon) - \beta\right] \\
&= (X'X + \lambda I)^{-1}X'X\beta + (X'X + \lambda I)^{-1}\underbrace{\mathbb{E}[X'\varepsilon]}_{0} - \beta \\
&= (X'X + \lambda I)^{-1}\left[(X'X + \lambda I)\beta - \lambda\beta\right] - \beta \\
&= \beta - \lambda(X'X + \lambda I)^{-1}\beta - \beta \\
&= -\lambda(X'X + \lambda I)^{-1}\beta
\end{aligned}$$

Calculating the Variance of Ridge Regression

X fixed (or condition or X)

$$
\begin{aligned}
\text{Var}(\widetilde{\beta}_\lambda) &= \text{Var}\left[(X'X + \lambda I)^{-1} X'(X\beta + \varepsilon)\right] \\
&= \text{Var}\left[(X'X + \lambda I)^{-1} X'\varepsilon\right] \\
&= \mathbb{E}\left[\left\{(X'X + \lambda I)^{-1} X'\varepsilon\right\}\left\{(X'X + \lambda I)^{-1} X'\varepsilon\right\}'\right] \\
&= \left[(X'X + \lambda I)^{-1} X'\right] \underbrace{\mathbb{E}[\varepsilon\varepsilon']}_{\sigma^2 I} \left[(X'X + \lambda I)^{-1} X'\right]' \\
&= \sigma^2 (X'X + \lambda I)^{-1} X'X \left(X'X + \lambda I\right)^{-1}
\end{aligned}
$$

For λ Sufficiently Small, MSE(OLS)>MSE(Ridge)

$$\begin{aligned}
\text{MSE}(\widehat{\beta}) - \text{MSE}(\widetilde{\beta}_\lambda) &= \left\{\text{Bias}^2(\widehat{\beta}) + \text{Var}(\widehat{\beta})\right\} - \left\{\text{Bias}^2(\widetilde{\beta}_\lambda) + \text{Var}(\widetilde{\beta}_\lambda)\right\} \\
&\vdots \\
&= \lambda \underbrace{(X'X + \lambda I)^{-1}}_{M'} \underbrace{\left[\sigma^2 \left\{2I + \lambda(X'X)^{-1}\right\} - \lambda\beta\beta'\right]}_{A} \underbrace{(X'X + \lambda I)^{-1}}_{M}
\end{aligned}$$

- $\lambda > 0$ and M is symmetric
- M is full rank $\implies Mv \neq 0$ unless $v = 0$
- $\implies v'[\lambda M'AM]v = \lambda(Mv)'A(Mv)$
- MSE(OLS) - MSE(Ridge) is PD iff M is PD
- To ensure M is PD, make λ small, e.g. $0 < \lambda < 2\sigma^2/\beta'\beta$

Lecture #8 – High-Dimensional Regression II

LASSO

Least Absolute Shrinkage and Selection Operator (LASSO)

Bühlmann & van de Geer (2011); Hastie, Tibshirani & Wainwright (2015)

Assume that X has been centered: don't penalize intercept!

Notation

$||\beta||_2^2 = \sum_{j=1}^p \beta_j^2, \quad ||\beta||_1 = \sum_{j=1}^p |\beta_j|$

Ridge Regression – L_2 Penalty

$$\widehat{\beta}_{Ridge} = \arg\min_{\beta} \, (\mathbf{y} - X\beta)'(\mathbf{y} - X\beta) + \lambda \, ||\beta||_2^2$$

LASSO – L_1 Penalty

$$\widehat{\beta}_{Lasso} = \arg\min_{\beta} \, (\mathbf{y} - X\beta)'(\mathbf{y} - X\beta) + \lambda \, ||\beta||_1$$

Other Ways of Thinking about LASSO

Constrained Optimization

$\arg\min_{\beta} (\mathbf{y} - X\beta)'(\mathbf{y} - X\beta) \quad \text{subject to} \quad \sum_{j=1}^{p} |\beta_j| \leq t$

Data-dependent, one-to-one mapping between λ and t.

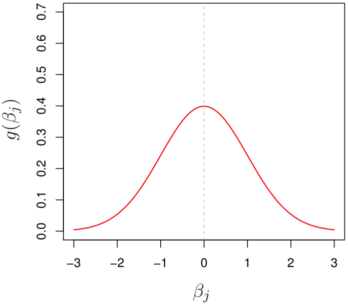
Bayesian Posterior Mode

Ignoring the intercept, LASSO is the posterior *mode* for β under

$$\mathbf{y}|X, \beta, \sigma^2 \sim N(X\beta, \sigma^2 I_n), \quad \beta \sim \prod_{j=1}^{p} \text{Lap}(\beta_j|0, \tau)$$

where $\lambda = 1/\tau$ and $\text{Lap}(x|\mu, \tau) = (2\tau)^{-1} \exp\left\{-\tau^{-1}|x - \mu|\right\}$

Comparing Ridge and LASSO – Bayesian Posterior Modes



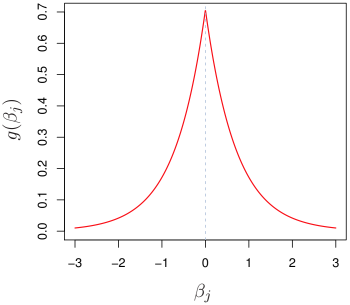


Figure: Ridge, at left, puts a normal prior on β while LASSO, at right, uses a Laplace prior, which has fatter tails and a taller peak at zero.

Comparing LASSO and Ridge – Constrained OLS

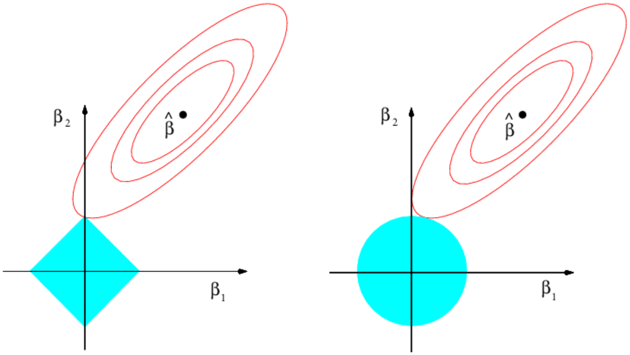


Figure: $\widehat{\beta}$ denotes the MLE and the ellipses are the contours of the likelihood. LASSO, at left, and Ridge, at right, both shrink β away from the MLE towards zero. Because of its diamond-shaped constraint set, however, LASSO favors a sparse solution while Ridge does not

No Closed-Form for LASSO!

Simple Special Case

Suppose that $X'X = I_p$

Maximum Likelihood

$$\widehat{\boldsymbol{\beta}}_{MLE} = (X'X)^{-1}X'\mathbf{y} = X'\mathbf{y}, \quad \widehat{\beta}_j^{MLE} = \sum_{i=1}^n x_{ij}y_i$$

Ridge Regression

$$\widehat{\boldsymbol{\beta}}_{Ridge} = (X'X + \lambda I_p)^{-1}X'\mathbf{y} = [(1+\lambda)I_p]^{-1}\,\widehat{\boldsymbol{\beta}}_{MLE}, \quad \widehat{\beta}_j^{Ridge} = \frac{\widehat{\beta}_j^{MLE}}{1+\lambda}$$

So what about LASSO?

LASSO when $X'X = I_p$ so $\widehat{\beta}_{MLE} = X'\mathbf{y}$

Want to Solve

$$\widehat{\boldsymbol{\beta}}_{LASSO} = \arg\min_{\boldsymbol{\beta}} (\mathbf{y} - X\boldsymbol{\beta})'(\mathbf{y} - X\boldsymbol{\beta}) + \lambda \left|\left|\boldsymbol{\beta}\right|\right|_1$$

Expand First Term

$$\begin{aligned}(\mathbf{y} - X\boldsymbol{\beta})'(\mathbf{y} - X\boldsymbol{\beta}) &= \mathbf{y}'\mathbf{y} - 2\boldsymbol{\beta}'X'\mathbf{y} + \boldsymbol{\beta}'X'X\boldsymbol{\beta} \\ &= (\text{constant}) - 2\boldsymbol{\beta}'\widehat{\boldsymbol{\beta}}_{MLE} + \boldsymbol{\beta}'\boldsymbol{\beta}\end{aligned}$$

Hence

$$\begin{aligned}\widehat{\boldsymbol{\beta}}_{LASSO} &= \arg\min_{\boldsymbol{\beta}} (\boldsymbol{\beta}'\boldsymbol{\beta} - 2\boldsymbol{\beta}'\widehat{\boldsymbol{\beta}}_{MLE}) + \lambda \left|\left|\boldsymbol{\beta}\right|\right|_1 \\ &= \arg\min_{\boldsymbol{\beta}} \sum_{j=1}^{p} \left(\beta_j^2 - 2\beta_j\widehat{\beta}_j^{MLE} + \lambda \left|\beta_j\right|\right)\end{aligned}$$

LASSO when $X'X = I_p$

Preceding Slide

$$\widehat{\boldsymbol{\beta}}_{LASSO} = \underset{\boldsymbol{\beta}}{\arg\min} \sum_{j=1}^{p} \left(\beta_j^2 - 2\beta_j \widehat{\beta}_j^{MLE} + \lambda \left|\beta_j\right|\right)$$

Key Simplification

Equivalent to solving j independent optimization problems:

$$\widehat{\beta}_j^{Lasso} = \underset{\beta_j}{\arg\min} \left(\beta_j^2 - 2\beta_j \widehat{\beta}_j^{MLE} + \lambda \left|\beta_j\right|\right)$$

- Sign of β_j^2 and $\lambda|\beta_j|$ unaffected by $\text{sign}(\beta_j)$
- $\widehat{\beta}_j^{MLE}$ is a function of data only – outside our control
- Minimization requires matching $\text{sign}(\beta_j)$ to $\text{sign}(\widehat{\beta}_j^{MLE})$

LASSO when $X'X = I_p$

Case I: $\widehat{\beta}^{MLE} > 0 \implies \beta_j > 0 \implies |\beta_j| = \beta_j$

Optimization problem becomes

$$\widehat{\beta}_j^{Lasso} = \arg\min_{\beta_j} \beta_j^2 - 2\beta_j \widehat{\beta}_j^{MLE} + \lambda \beta_j$$

Interior solution:

$$\beta_j^* = \widehat{\beta}_j^{MLE} - \frac{\lambda}{2}$$

Can't have $\beta_j < 0$: corner solution sets $\beta_j = 0$

$$\widehat{\beta}_j^{Lasso} = \max\left\{0, \widehat{\beta}_j^{MLE} - \frac{\lambda}{2}\right\}$$

LASSO when $X'X = I_p$

Case II: $\widehat{\beta}^{MLE} \leq 0 \implies \beta_j \leq 0 \implies |\beta_j| = -\beta_j$

Optimization problem becomes

$$\widehat{\beta}_j^{Lasso} = \arg\min_{\beta_j} \beta_j^2 - 2\beta_j \widehat{\beta}_j^{MLE} - \lambda\beta_j$$

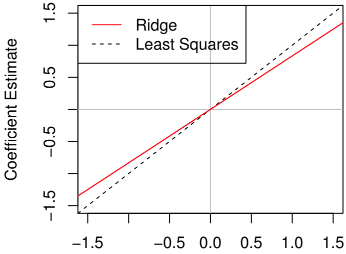
Interior solution:

$$\widehat{\beta}_j = \widehat{\beta}_j^{MLE} + \frac{\lambda}{2}$$

Can't have $\beta_j > 0$: corner solution sets $\beta_j = 0$

$$\widehat{\beta}_j^{Lasso} = \min\left\{0, \widehat{\beta}_j^{MLE} + \frac{\lambda}{2}\right\}$$

Ridge versus LASSO when $X'X = I_p$



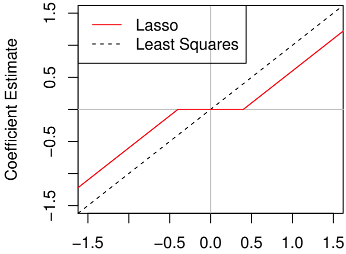


Figure: Horizontal axis in each plot is MLE

$$\widehat{\beta}_j^{Ridge} = \left(\frac{1}{1+\lambda}\right)\widehat{\beta}_j^{MLE}$$

$$\widehat{\beta}_j^{Lasso} = \text{sign}\left(\widehat{\beta}_j^{MLE}\right)\max\left\{0, \left|\widehat{\beta}_j^{MLE}\right| - \frac{\lambda}{2}\right\}$$

Calculating LASSO – The Shooting Algorithm

Cyclic Coordinate Descent

Data: $\mathbf{y}$, X, $\lambda \geq 0$, $\varepsilon > 0$

Result: LASSO Solution

$\boldsymbol{\beta} \leftarrow \text{ridge}(X, \mathbf{y}, \lambda)$

repeat

  $\boldsymbol{\beta}^{prev} \leftarrow \boldsymbol{\beta}$

  for $j = 1, \ldots, p$ **do**

    $a_j \leftarrow 2 \sum_i x_{ij}^2$

    $c_j \leftarrow 2 \sum_i x_{ij}(y_i - \mathbf{x}_i' \beta + \beta_j x_{ij})$

    $\beta_j \leftarrow \text{sign}(c_j/a_j) \max\{0, |c_j/a_j| - \lambda/a_j\}$

  end

until $|\boldsymbol{\beta} - \boldsymbol{\beta}^{prev}| < \varepsilon$;

Coordinate Updates in the Shooting Algorithm

$$\frac{\partial}{\partial \beta_j} (\mathbf{y} - X\boldsymbol{\beta})' (\mathbf{y} - X\boldsymbol{\beta}) = a_j \beta_j - c_j$$

$$a_j \equiv 2 \sum_{i=1}^{n} x_{ij}^2$$

$$c_j \equiv 2 \sum_{i=1}^{n} x_{ij} \Big(\underbrace{y_i - \mathbf{x}_i' \boldsymbol{\beta} + \beta_j x_{ij}}_{\text{Residual excluding } x_{ij}} \Big)$$

$$\beta_j^{\text{New}} = \begin{cases} (c_j + \lambda)/a_j, & c_j < -\lambda \\ 0, & c_j \in [-\lambda, \lambda] \\ (c_j - \lambda)/a_j, & c_j > \lambda \end{cases}$$

Prediction Error of LASSO

Punchline

With the appropriate choice of λ, Lasso can make very good predictions even when p is much larger than n, so long as $\sum_{j=1}^{p} |\beta_j|$ is small.

Sparsity?

One way to have small $\sum_{j=1}^{p} |\beta_j|$ is if $\boldsymbol{\beta}$ is *sparse*, i.e. $\beta_j = 0$ for most j, but sparsity is not required.

We'll look at a simple example...

Prediction Error of LASSO: Simple Example

Suppose that:

- X and $\mathbf{y}$ are centered
- X is fixed and scaled so that $\mathbf{x}_j'\mathbf{x}_j = n$
- $\mathbf{y} = X\boldsymbol{\beta}_0 + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim N(0, \sigma^2 I)$.
- $\lambda = c\sigma\sqrt{\log(p)/n}$ where c is a constant

Theorem

Let $\widehat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}}{\arg\min} \frac{1}{2n} \|\mathbf{y} - X\boldsymbol{\beta}\|_2^2 + \lambda \|\boldsymbol{\beta}_0\|_1$. Then,

$$\mathbb{P}\left(\frac{1}{n}\left\|X\boldsymbol{\beta}_{\mathbf{0}} - X\widehat{\boldsymbol{\beta}}\right\|_2^2 \leq 4\lambda\|\boldsymbol{\beta}_0\|_1\right) \geq 1 - p^{-(c^2/2-1)}$$

What Does This Mean?

$$\boxed{\mathbb{P}\left(\frac{1}{n}\left\|X\boldsymbol{\beta_0} - X\widehat{\boldsymbol{\beta}}\right\|_2^2 \leq 4\lambda \left\|\boldsymbol{\beta}_0\right\|_1\right) \geq 1 - p^{-(c^2/2-1)}}$$

Notation

$\|\mathbf{z}\|_2^2 \equiv \mathbf{z}'\mathbf{z}, \quad \|\boldsymbol{\alpha}\|_1 \equiv \sum_{j=1}^p |\alpha_j|$

Convenient Scaling

Divide RSS by $2n$: $\quad \widehat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \dfrac{1}{2n}\|\mathbf{y} - X\boldsymbol{\beta}\|_2^2 + \lambda\|\boldsymbol{\beta}\|_1$

Prediction Error Comparison

Optimal: $\boldsymbol{\varepsilon} = \mathbf{y} - X\boldsymbol{\beta}_0$ $\quad$ Lasso: $\widehat{\boldsymbol{\varepsilon}} = \boldsymbol{y} - X\widehat{\boldsymbol{\beta}}$

$$\frac{1}{n}\|\widehat{\boldsymbol{\varepsilon}} - \boldsymbol{\varepsilon}\|_2^2 = \frac{1}{n}\left\|(\mathbf{y} - X\widehat{\boldsymbol{\beta}}) - (\mathbf{y} - X\boldsymbol{\beta_0})\right\|_2^2 = \frac{1}{n}\left\|X\boldsymbol{\beta_0} - X\widehat{\boldsymbol{\beta}}\right\|_2^2$$

What Does This Mean?

$$\boxed{\mathbb{P}\left(\frac{1}{n}\left\|X\boldsymbol{\beta_0} - X\widehat{\boldsymbol{\beta}}\right\|_2^2 \leq 4\lambda\left\|\boldsymbol{\beta}_0\right\|_1\right) \geq 1 - p^{-(c^2/2-1)}}$$

Recall

$$\lambda = c\sigma\sqrt{\log(p)/n}, \quad \varepsilon \sim N(0, \sigma^2 I)$$

We choose c

Larger $c \implies$ higher probability that the bound obtains:

$$c = 2 \implies 1 - p^{-(c^2/2-1)} = 1 - 1/p$$

$$c = 3 \implies 1 - p^{-(c^2/2-1)} = 1 - p^{-7/2}$$

$$c = 4 \implies 1 - p^{-(c^2/2-1)} = 1 - p^{-7}$$

What Does This Mean?

$$\boxed{\mathbb{P}\left(\frac{1}{n}\left\|X\boldsymbol{\beta_0} - X\widehat{\boldsymbol{\beta}}\right\|_2^2 \leq 4\lambda \left\|\boldsymbol{\beta}_0\right\|_1\right) \geq 1 - p^{-(c^2/2-1)}}$$

Recall

$\lambda = c\sigma\sqrt{\log(p)/n}, \quad \varepsilon \sim N(0, \sigma^2 I)$

We choose c

Larger $c \implies$ looser bound:

$$c = 2 \implies 4\lambda \left\|\boldsymbol{\beta}_0\right\|_1 = 8\sigma\sqrt{\log(p)/n} \times \left\|\boldsymbol{\beta}_0\right\|_1$$
$$c = 3 \implies 4\lambda \left\|\boldsymbol{\beta}_0\right\|_1 = 12\sigma\sqrt{\log(p)/n} \times \left\|\boldsymbol{\beta}_0\right\|_1$$
$$c = 4 \implies 4\lambda \left\|\boldsymbol{\beta}_0\right\|_1 = 16\sigma\sqrt{\log(p)/n} \times \left\|\boldsymbol{\beta}_0\right\|_1$$

We can allow $p \gg n$ provided $\|\beta\|_1$ is small

$$\boxed{\mathbb{P}\left(\frac{1}{n}\left\|X\boldsymbol{\beta_0} - X\widehat{\beta}\right\|_2^2 \leq 4\lambda\left\|\boldsymbol{\beta}_0\right\|_1\right) \geq 1 - p^{-(c^2/2-1)}}$$

Recall

$\lambda = c\sigma\sqrt{\log(p)/n}, \quad \varepsilon \sim N(0, \sigma^2 I)$

p	n	$\sqrt{\log(p)/n}$
100	100	0.21
1000	1000	0.08
1000	100	0.26
10000	1000	0.10
10000	100	0.30
100000	1000	0.11

Lecture #9 – High-Dimensional Regression III

Principal Component Analysis (PCA)

Principal Components Regression

Comparing OLS, Ridge, and PCR

Overview of Factor Models

Choosing the Number of Factors

Diffusion Index Forecasting

Principal Component Analysis (PCA)

Notation

Let $\mathbf{x}$ be a $p \times 1$ random vector with variance-covariance matrix Σ.

Optimization Problem

$$\boldsymbol{\alpha}_1 = \underset{\boldsymbol{\alpha}}{\arg\max}\ \text{Var}(\boldsymbol{\alpha}'\mathbf{x}) \quad \text{subject to} \quad \boldsymbol{\alpha}'\boldsymbol{\alpha} = 1$$

First Principal Component

The linear combination $\boldsymbol{\alpha}_1'\mathbf{x}$ is the first principal component of $\mathbf{x}$.

The random vector $\mathbf{x}$ has maximal variation in the direction α_1.

Solving for $\boldsymbol{\alpha}_1$

Lagrangian

$$\mathcal{L}(\boldsymbol{\alpha}_1, \lambda) = \boldsymbol{\alpha}'\Sigma\boldsymbol{\alpha} - \lambda(\boldsymbol{\alpha}'\boldsymbol{\alpha} - 1)$$

First Order Condition

$$2(\Sigma\boldsymbol{\alpha}_1 - \lambda\boldsymbol{\alpha}_1) = 0 \iff (\Sigma - \lambda I_p)\boldsymbol{\alpha}_1 = 0 \iff \Sigma\boldsymbol{\alpha}_1 = \lambda\boldsymbol{\alpha}_1$$

Variance of 1st PC

$\boldsymbol{\alpha}_1$ is an e-vector of Σ but which one? Substituting,

$$\text{Var}(\boldsymbol{\alpha}_1'\mathbf{x}) = \boldsymbol{\alpha}_1'(\Sigma\boldsymbol{\alpha}_1) = \lambda\boldsymbol{\alpha}_1'\boldsymbol{\alpha}_1 = \lambda$$

Solution

Var. of 1st PC equals λ and this is what we want to maximize, so $\boldsymbol{\alpha}_1$ is the e-vector corresponding to the largest e-value.

Subsequent Principal Components

Additional Constraint

Construct 2nd PC by solving the same problem as before with the additional constraint that $\boldsymbol{\alpha}_2'\mathbf{x}$ is uncorrelated with $\boldsymbol{\alpha}_1'\mathbf{x}$.

*j*th Principal Component

The linear combination $\boldsymbol{\alpha}_j'\mathbf{x}$ where $\boldsymbol{\alpha}_j$ is the e-vector corresponding to the jth largest e-value of Σ.

Sample PCA

Notation

$X = (n \times p)$ centered data matrix – columns are mean zero.

SVD

$X = UDV'$, thus $X'X = VDU'UDV' = VD^2V'$

Sample Variance Matrix

$S = n^{-1}X'X$ has same e-vectors as $X'X$ – the columns of V!

Sample PCA

Let $\mathbf{v}_j$ be the jth column of V. Then,

$$\begin{aligned} \mathbf{v}_j &= \text{PC loadings for jth PC of } S \\ \mathbf{v}_j'\mathbf{x}_i &= \text{PC score for individual/time period } i \end{aligned}$$

Sample PCA

PC scores for jth PC

$$\mathbf{z}_j = \begin{bmatrix} z_{j1} \\ \vdots \\ z_{jn} \end{bmatrix} = \begin{bmatrix} \mathbf{v}_j'\mathbf{x}_1 \\ \vdots \\ \mathbf{v}_j'\mathbf{x}_n \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1'\mathbf{v}_j \\ \vdots \\ \mathbf{x}_n'\mathbf{v}_j \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1' \\ \vdots \\ \mathbf{x}_n' \end{bmatrix} \mathbf{v}_j = X\mathbf{v}_j$$

Getting PC Scores from SVD

Since $X = UDV'$ and $V'V = I$, $XV = UD$, i.e.

$$\begin{bmatrix} \mathbf{x}_1' \\ \vdots \\ \mathbf{x}_n' \end{bmatrix} \begin{bmatrix} \mathbf{v}_i & \cdots & \mathbf{v}_p \end{bmatrix} = \begin{bmatrix} \mathbf{u}_1 & \cdots & \mathbf{u}_r \end{bmatrix} \begin{bmatrix} d_1 & \cdots & 0 \\ & \ddots & \\ 0 & \cdots & d_r \end{bmatrix}$$

Hence we see that $\mathbf{z}_j = d_j \mathbf{u}_j$

Properties of PC Scores $\mathbf{z}_j$

Since X has been de-meaned:

$$\bar{z}_j = \frac{1}{n}\sum_{i=1}^{n} \mathbf{v}_j'\mathbf{x}_i = \mathbf{v}_j'\left(\frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i\right) = \mathbf{v}_j'\mathbf{0} = 0$$

Hence, since $X'X = VD^2V'$

$$\frac{1}{n}\sum_{i=1}^{n}(z_{ji}-\bar{z}_j)^2 = \frac{1}{n}\sum_{i=1}^{n} z_{ji}^2 = \frac{1}{n}\mathbf{z}_j'\mathbf{z}_j = \frac{1}{n}\left(X\mathbf{v}_j\right)'\left(X\mathbf{v}_j\right) = \mathbf{v}_j'S\mathbf{v}_j = d_j^2/n$$

Principal Components Regression (PCR)

1. Start with centered X and $\mathbf{y}$.
2. SVD of $X \implies$ PC scores: $\mathbf{z}_j = X\mathbf{v}_j = d_j\mathbf{u}_j$.
3. Regress $\mathbf{y}$ on $\begin{bmatrix} \mathbf{z}_1 & \dots & \mathbf{z}_m \end{bmatrix}$ where $m < p$.

$$\widehat{\mathbf{y}}_{\text{PCR}}(m) = \sum_{j=1}^{m} \mathbf{z}_j \widehat{\theta}_j, \quad \widehat{\theta}_j = \frac{\mathbf{z}_j'\mathbf{y}}{\mathbf{z}_j'\mathbf{z}_j} \quad \text{(PCs orthogonal)}$$

Standardizing X

Because PCR is not scale invariant, it is common to standardize X.

This amounts to PCA performed on a correlation matrix.

Comparing PCR, OLS and Ridge Predictions

Assumption

Centered data matrix $\underset{(n\times p)}{X}$ with rank p so OLS estimator is unique.

SVD

$$\underset{(n\times p)}{X} = \underset{(n\times p)}{U}\underset{(p\times p)}{D}\underset{(p\times p)}{V'}, \quad U'U = V'V = I_p, \quad VV' = I_p$$

Ridge Predictions

$$\begin{aligned}
\widehat{\mathbf{y}}_{\text{Ridge}}(\lambda) &= X\widehat{\beta}_{\text{Ridge}}(\lambda) = X\left(X'X + \lambda I_p\right)^{-1} X'\mathbf{y} \\
&= \left[UD\left(D^2 + \lambda I_p\right)^{-1} DU'\right]\mathbf{y} \\
&= \sum_{j=1}^{p}\left(\frac{d_j^2}{d_j^2 + \lambda}\right)\mathbf{u}_j\mathbf{u}_j'\mathbf{y}
\end{aligned}$$

Relating OLS and Ridge to PCR

Recall: U is Orthonormal

$$\mathbf{u}_j\mathbf{u}_j'\mathbf{y} = d_j\mathbf{u}_j\left(d_j^2\mathbf{u}_j'\mathbf{u}_j\right)^{-1}d_j\mathbf{u}_j'\mathbf{y} = \mathbf{z}_j(\mathbf{z}_j'\mathbf{z}_j)^{-1}\mathbf{z}_j'\mathbf{y} = \mathbf{z}_j\widehat{\theta}_j$$

Substituting

$$\widehat{\mathbf{y}}_{\text{Ridge}}(\lambda) = \sum_{j=1}^{m}\left(\frac{d_j^2}{d_j^2+\lambda}\right)\mathbf{u}_j\mathbf{u}_j'\mathbf{y} = \sum_{j=1}^{m}\left(\frac{d_j^2}{d_j^2+\lambda}\right)\mathbf{z}_j\widehat{\theta}_j$$

$$\widehat{\mathbf{y}}_{\text{OLS}} = \widehat{\mathbf{y}}_{\text{Ridge}}(0) = \sum_{j=1}^{p}\mathbf{z}_j\widehat{\theta}_j$$

Comparing PCR, OLS, and Ridge Predictions

$$\widehat{\mathbf{y}}_{\text{PCR}}(m) = \sum_{j=1}^{m} \mathbf{z}_j \widehat{\theta}_j, \quad \widehat{\mathbf{y}}_{\text{OLS}} = \sum_{j=1}^{p} \mathbf{z}_j \widehat{\theta}_j, \quad \widehat{\mathbf{y}}_{\text{Ridge}}(\lambda) = \sum_{j=1}^{m} \left(\frac{d_j^2}{d_j^2 + \lambda} \right) \mathbf{z}_j \widehat{\theta}_j$$

- $\mathbf{z}_j$ is the jth sample PC
- d_j^2/n is the variance of the jth sample PC
- Ridge regresses y on sample PCs but shrinks predictions towards zero: higher variance PCs are shrunk less.
- PCR truncates the PCs with the smallest variance.
- OLS neither shrinks nor truncates: is uses all the PCs.

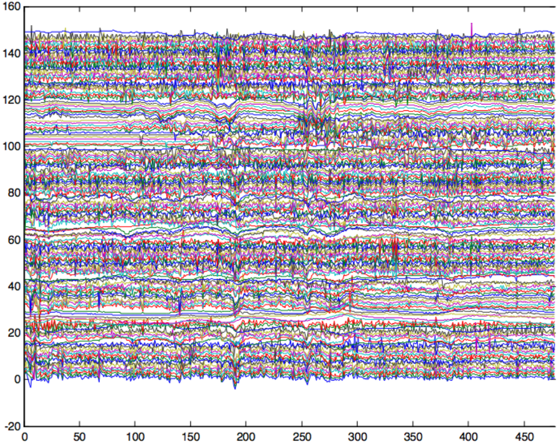
The Basic Idea

- $(T \times N)$ Matrix X of observations
- X_t contains a large number N of time series
- Comparable number T of time periods
- Can we "summarize" this information in some useful way?
- Forecasting and policy analysis applications

Survey Articles

Stock & Watson (2010), Bai & Ng (2008), Stock & Watson (2006)

Example: Stock and Watson Dataset



Monthly Macroeconomic Indicators: $N > 200$, $T > 400$

Classical Factor Analysis Model

Assume that X_t has been de-meaned...

$$\underset{(N\times 1)}{X_t} = \Lambda \underset{(r\times 1)}{F_t} + \epsilon_t$$

$$\begin{bmatrix} F_t \\ \epsilon_t \end{bmatrix} \overset{iid}{\sim} \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} I_r & 0 \\ 0 & \Psi \end{bmatrix} \right)$$

$\Lambda =$ matrix of factor loadings

$\Psi =$ diagonal matrix of idiosyncratic variances.

Adding Time-Dependence

$$\underset{(N\times 1)}{X_t} = \Lambda \underset{(r\times 1)}{F_t} + \epsilon_t$$

$$\underset{(r\times 1)}{F_t} = A_1 F_{t-1} + \ldots + A_p F_{t-p} + u_t$$

$$\begin{bmatrix} u_t \\ \epsilon_t \end{bmatrix} \overset{iid}{\sim} \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} I_r & 0 \\ 0 & \Psi \end{bmatrix} \right)$$

Terminology

Static	X_t depends only on F_t
Dynamic	X_t depends on lags of F_t as well
Exact	Ψ is diagonal and ϵ_t independent over time
Approximate	Some cross-sectional & temporal dependence in ϵ_t

The model I wrote down on the previous slide is sometimes called an "exact, static factor model" even though F_t has dynamics.

Some Caveats

1. Are “static” and “dynamic” really different?
   - Can write dynamic model as a static one with more factors
   - Static representation involves “different” factors, but we may not care: are the factors “real” or just a data summary?
2. Can we *really* allow for cross-sectional dependence?
   - Unless the off-diagonal elements of Ψ are close to zero we can't tell them apart from the common factors
   - “Approximate” factor models basically assume conditions under which the off-diagonal elements of Ψ are negligible
   - Similarly, time series dependence in ϵ_t can't be very strong (stationary ARMA is ok)

Methods of Estimation for Dynamic Factor Models

1. Bayesian Estimation
2. Maximum Likelihood: EM-Algorithm + Kalman Filter
   - Watson & Engle (1983); Ghahramani & Hinton (1996); Jungbacker & Koopman (2008); Doz, Giannone & Reichlin (2012)
3. "Nonparametric" Estimation via PCA
   - PCA on the $(T \times N)$ matrix X, ignoring time dependence.
   - The $(r \times 1)$ vector $\widehat{F}_t$ of PC scores associated with the first r PCs are our estimate of F_t
   - Essentially treats F_t as an r-dimensional *parameter* to be estimated from an N-dimensional observation X_t

Estimation by PCA

PCA Normalization

- $F'F/T = I_r$ where $F = (F_1, \dots, F_T)'$
- $\Lambda'\Lambda = \text{diag}(\mu_1, \dots, \mu_r)$ where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_r$

Assumption I

Factors are *pervasive*: $\Lambda'\Lambda/N \to D_\Lambda$ an $(r \times r)$ full rank matrix.

Assumption II

max e-value $E[\epsilon_t \epsilon_t'] \leq c \leq \infty$ for all N.

Upshot of the Assumptions

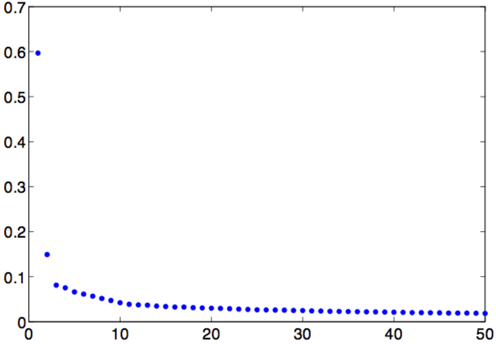
Average over the cross-section $\implies$ contribution from the factors persists while contribution from the idiosyncratic terms disappears as $N \to \infty$.

Key Result for PCA Estimation

Under the assumptions on the previous slide and some other technical conditions, the first r PCs of X consistently estimate the space spanned by the factors as $N, T \to \infty$.

Choosing the Number of Factors – Scree Plot

If we use PC estimation, we can look a something called a "scree plot" to help us decide how many PCs to include:



This figure depicts the eigenvalues for an $N = 1148$, $T = 252$ dataset of excess stock returns

Choosing the Number of Factors – Bai & Ng (2002)

Choose r to minimize an information criterion:

$$IC(r) = \log V_r(\widehat{\Lambda}, \widehat{F}) + r \cdot g(N, T)$$

where

$$V_r(\Lambda, F) = \frac{1}{NT} \sum_{t=1}^{T} (X_t - \Lambda F_t)'(X_t - \Lambda F_t)$$

and g is a penalty function. The paper provides conditions on the penalty function that guarantee consistent estimation of the "true number" of factors.

Some Special Problems in High-dimensional Forecasting

Estimation Uncertainty

We've already seen that OLS can perform very badly if the number of regressors is large relative to sample size.

Best Subsets Infeasible

With more than 30 or so regressors, we can't check all subsets of predictors making classical model selection problematic.

Noise Accumulation

Large N is supposed to help in factor models: averaging over the cross-section gives a consistent estimator of factor space. This can fail in practice, however, since it relies on the assumption that the factors are *pervasive*. See Boivin & Ng (2006).

Diffusion Index Forecasting – Stock & Watson (2002a,b)

JASA paper has the theory, JBES paper has macro forecasting example.

Basic Setup

Forecast scalar time series y_{t+1} using N-dimensional collection of time series X_t where we observe periods $t = 1, \ldots, T$.

Assumption

Static representation of Dynamic Factor Model:

$$\begin{aligned} y_t &= \beta' F_t + \gamma(L) y_t + \epsilon_{t+1} \\ X_t &= \Lambda F_t + e_t \end{aligned}$$

"Direct" Multistep Ahead Forecasts

"Iterated" forecast would be linear in F_t, y_t and lags:

$$y_{t+h}^h = \alpha_h + \beta_h(L) F_t + \gamma_h(L) y_t + \epsilon_{t+h}^h$$

This is really just PCR

Diffusion Index Forecasting – Stock & Watson (2002a,b)

Estimation Procedure

1. Data Pre-processing
   1.1 Transform all series to stationarity (logs or first difference)
   1.2 Center and standardize all series
   1.3 Remove outliers (ten times IQR from median)
   1.4 Optionally augment X_t with lags
2. Estimate the Factors
   - No missing observations: PCA on X_t to estimate $\widehat{F}_t$
   - Missing observations/Mixed-frequency: EM-algorithm
3. Fit the Forecasting Regression
   - Regress y_t on a constant and lags of $\widehat{F}_t$ and y_t to estimate the parameters of the "Direct" multistep forecasting regression.

Diffusion Index Forecasting – Stock & Watson (2002b)

Recall from above that, under certain assumptions, PCA consistently estimates the space spanned by the factors. Broadly similar assumptions are at work here.

Main Theoretical Result

Moment restrictions on (ϵ, e, F) plus a "rank condition" on Λ imply that the MSE of the procedure on the previous slide converges to that of the infeasible optimal procedure, provided that $N, T \to \infty$.

Diffusion Index Forecasting – Stock & Watson (2002a)

Forecasting Experiment

- Simulated real-time forecasting of eight monthly macro variables from 1959:1 to 1998:12
- Forecasting Horizons: 6, 12, and 24 months
- "Training Period" 1959:1 through 1970:1
- Predict *h*-steps ahead out-of-sample, roll and re-estimate.
- BIC to select lags and # of Factors in forecasting regression
- Compare Diffusion Index Forecasts to Benchmark
  - AR only
  - Factors only
  - AR + Factors

Diffusion Index Forecasting – Stock & Watson (2002a)

Empirical Results

- Factors provide a substantial improvement over benchmark forecasts in terms of MSPE
- Six factors explain 39% of the variance in the 215 series; twelve explain 53%
- Using all 215 series tends to work better than restricting to balanced panel of 149 (PCA estimation)
- Augmenting X_t with lags isn't helpful

Lecture #10 – Selective Inference

Optimal Inference After Model Selection (Fithian et al., 2017)

How Statistics is Done In Reality

Step 1: Selection – Decide what questions to ask.

"The analyst chooses a statistical model for the data at hand, and formulates testing, estimation, or other problems in terms of unknown aspects of that model."

Step 2: Inference – Answer the Questions.

"The analyst investigates the chosen problems using the data and the selected model."

Problem – "Data-snooping"

Standard techniques for (frequentist) statistical inference assume that we choose our questions before observing the data.

Simple Example: "File Drawer Problem"

$Y_i \sim \text{iid } \mathrm{N}(\mu_i, 1)$ for $i = 1, \ldots, n$

- I want to know which $\mu_i \neq 0$, but I'm busy and n is big.
- My RA looks at each Y_i and finds the "interesting" ones, namely $\widehat{\mathcal{I}} = \{i \colon |Y_i| > 1\}$.
- I test $H_{0,i} \colon \mu_i = 0$ against the two-sided alternative at the 5% significance level for each $i \in \widehat{\mathcal{I}}$.

Two Questions

1. What is the probability of falsely rejecting $H_{0,i}$?
2. Among all $H_{0,i}$ that I test, what fraction are false rejections?

Simple Example: "File Drawer Problem"

$$
\begin{aligned}
\mathbb{P}_{H_{0,i}}(\{\text{Reject } H_{0,i}\}) &= \mathbb{P}_{H_{0,i}}(\{\text{Test } H_{0,i}\} \cap \{\text{Reject } H_{0,i}\}) \\
&= \mathbb{P}_{H_{0,i}}(\{\text{Reject } H_{0,i}\} | \{\text{Test } H_{0,i}\}) \mathbb{P}_{H_{0,i}}(\{\text{Test } H_{0,i}\}) \\
&= \mathbb{P}_{H_{0,i}}\left(\{|Y_i| > 1.96\} | \{|Y_i| > 1\}\right) \mathbb{P}_{H_{0,i}}(\{|Y_i| > 1\}) \\
&= \frac{2\Phi(-1.96)}{2\Phi(-1)} \times 2\Phi(-1) \\
&\approx 0.16 \times 0.32 \approx 0.05
\end{aligned}
$$

$$
\begin{aligned}
\mathbb{P}_{H_{0,i}}(\{\text{Reject } H_{0,i}\} | \{\text{Test } H_{0,i}\}) &= \mathbb{P}_{H_{0,i}}\left(\{|Y_i| > 1.96\} | \{|Y_i| > 1\}\right) \\
&= \frac{\Phi(-1.96)}{\Phi(-1)} \approx 0.16
\end{aligned}
$$

Simple Example: "File Drawer Problem"

Conditional vs. Unconditional Type I Error Rates

- The conditional probability of falsely rejecting $H_{0,i}$, given that I have tested it, is about 0.16.
- The unconditional probability of falsely rejecting $H_{0,i}$ is 0.05 since I only test a false null with probability 0.32.

Idea for Post-Selection Inference

Control the Type I Error Rate conditional on selection: "The answer must be valid, given that the question was asked."

Simple Example: "File Drawer Problem"

Conditional Type I Error Rate

Solve $\mathbb{P}_{H_{0,i}}(\{|Y_i| > c\}|\{|Y_i| > 1\}) = 0.05$ for c.

$$\begin{aligned}\mathbb{P}_{H_{0,i}}(\{|Y_i| > c\}|\{|Y_i| > 1\}) &= \frac{\Phi(-c)}{\Phi(-1)} = 0.05 \\ c &= -\Phi^{-1}\big(\Phi(-1) \times 0.05\big) \\ c &\approx 2.41\end{aligned}$$

Notice:

To account for the first-stage selection step, we need a larger critical value: 2.41 vs. 1.96. This means the test is less powerful.

Selective Inference vs. Sample-Splitting

Classical Inference

Control the Type I error under model M: $\mathbb{P}_{M,H_0}(\text{reject } H_0) \leq \alpha$.

Selective Inference

Control the Type I error under model M, given that M and H_0 were selected: $\mathbb{P}_{M,H_0}\big(\text{reject } H_0 | \{M, H_0 \text{ selected}\}\big) \leq \alpha$.

Sample-Splitting

Use different datasets to choose (M, H_0) and carry out inference:
$\mathbb{P}_{M,H_0}\big(\text{reject } H_0 | \{M, H_0 \text{ selected}\}\big) = \mathbb{P}_{M,H_0}(\text{reject } H_0)$.

Selective Inference in Exponential Family Models

Questions

1. Recipe for selective inference in realistic examples?
2. How to construct the "best" selective test in a given example?
3. How does selective inference compare to sample-splitting?

Fithian, Sun & Taylor (2017)

- Use classical theory for exponential family models (Lehmann & Scheffé).
- Computational procedure for UMPU selective test/CI after arbitrary model/hypothesis selection.
- Sample-splitting is typically inadmissible (wastes information).
- Example: post-selection inference for high-dimensional regression

A Prototype Example of Selective Inference

This is my own example, but uses the same idea that underlies Fithian et al.

- Choose between two models on a parameter δ.
  - If $\delta \neq 0$, choose M1; if $\delta = 0$, choose M2
  - E.g. δ is the endogeneity of X, M1 is IV and M2 is OLS
- Observe $Y_\delta \sim N(\delta, \sigma_\delta^2)$ and use this to choose a model.
  - Selection Event: $A \equiv \{|Y_\delta| > c\}$, for some critical value c
  - If A, then choose M1. Otherwise, choose M2.
- After choosing a model, carry out inference for β.
  - Under a particular model M, $Y_\beta \sim N(\beta, \sigma_\beta^2)$
  - β is a *model-specific* parameter: could be meaningless or not even exist under a different model.
- If Y_β and Y_δ are correlated (under model M), we need to account for conditioning on A when carrying out inference for β.

All Calculations are Under a Given Model M

Key Idea

Under whichever model M ends up being selected, there is a joint normal distribution for Y_β and Y_δ *without* conditioning on A.

WLOG unit variances, ρ known

$$\begin{bmatrix} Y_\beta \\ Y_\delta \end{bmatrix} \sim \mathrm{N}\left(\begin{bmatrix} \beta \\ \delta \end{bmatrix}, \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix} \right)$$

As long as we can consistently estimate the variances of Y_β and Y_δ along with their covariance, this is not a problem.

Selective Inference in a Bivariate Normal Example

$$\boxed{\begin{bmatrix} Y_\beta \\ Y_\delta \end{bmatrix} \sim \mathrm{N}\left(\begin{bmatrix} \beta \\ \delta \end{bmatrix}, \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix} \right), \quad A \equiv \{|Y_\delta| > c\}}$$

Two Cases

1. Condition on A occurring
2. Condition on A *not* occurring

Problem

If δ were known, we could directly calculate how conditioning on A affects the distribution of Y_β, but δ is unknown!

Solution

Condition on a sufficient statistic for δ.

Conditioning on a Sufficient Statistic

Theorem

If U is a sufficient statistic for δ, then the joint distribution of (Y_β, Y_δ) given U does not depend on δ.

In Our Example

Residual $U = Y_\delta - \rho Y_\beta$ from a projection of Y_δ onto Y_β is sufficient for δ.

Straightforward Calculation

$$\left[\begin{array}{c} Y_\beta \\ Y_\delta \end{array}\right] \Bigg| (U = u) = \left[\begin{array}{c} \beta + Z \\ u + \rho(\beta + Z) \end{array}\right], \quad Z \sim \mathrm{N}(0,1)$$

Notice that this is a singular normal distribution

The Distribution of $Y_\beta|(A, U = u)$

$$\boxed{\left[\begin{array}{c} Y_\beta \\ Y_\delta \end{array}\right] \Bigg| (U = u) = \left[\begin{array}{c} \beta + Z \\ u + \rho(\beta + Z) \end{array}\right], \quad Z \sim \mathrm{N}(0, 1)}$$

Start with case in which A occurs so we select $M1$. Under $H_0\colon \beta = \beta_0$,

$$\begin{aligned} \mathbb{P}_{\beta_0}\left(Y_\beta \leq y | A, U = u\right) &= \frac{\mathbb{P}_{\beta_0}(\{Y_\beta \leq y\} \cap A | U = u)}{\mathbb{P}_{\beta_0}(A|U = u)} \\ &= \frac{\mathbb{P}\left(\{Z \leq y - \beta_0\} \cap \{|u + \rho(\beta_0 + Z)| > c\}\right)}{\mathbb{P}\left(|u + \rho(\beta_0 + Z)| > c\right)} \end{aligned}$$

$\mathbb{P}(A|U = u)$ under $H_0\colon \beta = \beta_0$

$$
\begin{aligned}
P_D(A) &\equiv P_{\beta_0}(A|U = u) \\
&= \mathbb{P}\left(|u + \rho(\beta_0 + Z)| > c\right) \\
&= \mathbb{P}\left[u + \rho(\beta_0 + Z) > c\right] + \mathbb{P}\left[u + \rho(\beta_0 + Z) < -c\right] \\
&= \mathbb{P}\left[\rho(\beta_0 + Z) > c - u\right] + \mathbb{P}\left[u + \rho(\beta_0 + Z) < -c - u\right] \\
&= 1 - \Phi\left(\frac{c - u}{\rho} - \beta_0\right) + \Phi\left(\frac{-c - u}{\rho} - \beta_0\right)
\end{aligned}
$$

$\mathbb{P}(\{Y_\beta \leq y\} \cap A | U = u)$ under $H_0\colon \beta = \beta_0$

$$
\begin{aligned}
P_N(A) &\equiv \mathbb{P}(\{Y_\beta \leq y\} \cap A | U = u) \\
&= \mathbb{P}\left(\{Z \leq y - \beta_0\} \cap \{|u + \rho(\beta_0 + Z)| > c\}\right) \\
&= \begin{cases}
\Phi\left(y - \beta_0\right), & y < (-c-u)/\rho \\
\Phi\left(\dfrac{-c-u}{\rho} - \beta_0\right), & (-c-u)/\rho \leq y \leq (c-u)/\rho \\
\Phi(y - \beta_0) - \Phi\left(\dfrac{c-u}{\rho} - \beta_0\right) + \Phi\left(\dfrac{-c-u}{\rho} - \beta_0\right), & y > (c-u)/\rho
\end{cases}
\end{aligned}
$$

$F_{\beta_0}(y|A, U = u)$

Define $\ell(u) = (-c - u)/\rho$, $r(u) = (c - u)/\rho$. We have:

$$F_{\beta_0}(y|A, U = u) = P_N(A)/P_D(A)$$

where

$$P_D(A) \equiv 1 - \Phi\left(r(u) - \beta_0\right) + \Phi\left(\ell(u) - \beta_0\right)$$

$$P_N(A) \equiv \begin{cases} \Phi\left(y - \beta_0\right), & y < \ell(u) \\ \Phi\left(\ell(u) - \beta_0\right), & \ell(u) \leq y \leq r(u) \\ \Phi(y - \beta_0) - \Phi\left(r(u) - \beta_0\right) + \Phi\left(\ell(u) - \beta_0\right), & y > r(u) \end{cases}$$

Note that $F_{\beta_0}(y|A, U = u)$ has a *flat region* where $\ell(u) \leq y \leq r(u)$

$Q_{\beta_0}(p|A, U = u)$

Inverting the CDF from the preceding slide:

$$Q_{\beta_0}(p|A, U = u) = \begin{cases} \beta_0 + \Phi^{-1}\left(p \times P_D(A)\right), & p < p^* \\ \beta_0 + \Phi^{-1}\left[p \times P_D(A) + \Phi\left(r(u) - \beta_0\right) - \Phi\left(\ell(u) - \beta_0\right)\right], & p \geq p^* \end{cases}$$

where

$$\begin{aligned} p^* &\equiv \Phi\left(\ell(u) - \beta_0\right)/P_D(A) \\ P_D(A) &\equiv 1 - \Phi\left(r(u) - \beta_0\right) + \Phi\left(\ell(u) - \beta_0\right) \\ \ell(u) &\equiv (-c - u)/\rho \\ r(u) &\equiv (c - u)/\rho \end{aligned}$$

The Distribution of $Y_\beta|(A^c, U = u)$

$$\boxed{\left[\begin{array}{c} Y_\beta \\ Y_\delta \end{array}\right]\Bigg|(U = u) = \left[\begin{array}{c} \beta + Z \\ u + \rho(\beta + Z) \end{array}\right], \quad Z \sim \mathrm{N}(0, 1)}$$

If A does not occur, when we select $M2$. Under $H_0\colon \beta = \beta_0$,

$$\begin{aligned} \mathbb{P}_{\beta_0}\left(Y_\beta \leq y|A^c, U = u\right) &= \frac{\mathbb{P}_{\beta_0}(\{Y_\beta \leq y\} \cap A^c|U = u)}{\mathbb{P}_{\beta_0}(A^c|U = u)} \\ &= \frac{\mathbb{P}\left(\{Z \leq y - \beta_0\} \cap \{|u + \rho(\beta_0 + Z)| < c\}\right)}{\mathbb{P}\left(|u + \rho(\beta_0 + Z)| < c\right)} \end{aligned}$$

$F_{\beta_0}(y|A^c, U = u)$

As above, define $\ell(u) = (-c - u)/\rho$, $r(u) = (c - u)/\rho$. We have:

$$F_{\beta_0}(y|A^c, U = u) = P_N(A^c)/P_D(A^c)$$

where

$$P_D(A^c) \equiv \Phi\left(r(u) - \beta_0\right) - \Phi\left(\ell(u) - \beta_0\right)$$

$$P_N(A^c) \equiv \begin{cases} 0, & y < \ell(u) \\ \Phi(y - \beta_0) - \Phi\left(\ell(u) - \beta_0\right), & \ell(u) \leq y \leq r(u) \\ \Phi\left(r(u) - \beta_0\right) - \Phi\left(\ell(u) - \beta_0\right), & y > r(u) \end{cases}$$

Notice that this is a CDF with a bounded support set: $y \in [\ell(u), r(u)]$

$Q_{\beta_0}(p|A^c, U = u)$

Inverting the CDF from the preceding slide:

$$Q_{\beta_0}(p|A^c, U = u) = \beta_0 + \Phi^{-1}\left[p \times P_D(A^c) + \Phi\left(\ell(u) - \beta_0\right)\right]$$

where:

$$\begin{aligned} P_D(A^c) &\equiv \Phi\left(r(u) - \beta_0\right) - \Phi\left(\ell(u) - \beta_0\right) \\ \ell(u) &\equiv (-c - u)/\rho \\ r(u) &\equiv (c - u)/\rho \end{aligned}$$

Equal-tailed Selective Test

Conditional on A

1. Compute observed value u of $U = Y_\delta - \rho Y_\beta$ (given A).
2. Compute $q_{\alpha/2} \equiv Q_{\beta_0}(\alpha/2|A, U = u)$
3. $q_{1-\alpha/2} \equiv Q_{\beta_0}(1 - \alpha/2|A, U = u)$
4. Reject $H_0\colon \beta = \beta_0$ if Y_β lies outside outside $\left[q_{\alpha/2}, q_{1-\alpha/2}\right]$.

Conditional on A^c

Same as above, but replace A with A^c in the preceding expressions.

Constructing a Confidence Interval

Simply invert the test: find the values of β_0 that are not rejected.

Valid *conditional* on $(U = u) \implies$ valid unconditionally!