Econ 722 – Advanced Econometrics IV

Francis J. DiTraglia

University of Pennsylvania

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

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

Bayes Risk and Maximum Risk

Comparing Risk

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

Maximum Risk

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

Bayes Risk

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

Bayes and Minimax Rules

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

Minimax Rule/Estimator

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

Bayes Rule/Estimator

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

Recall: Bayes' Theorem and Marginal Likelihood

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

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

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

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

Posterior Expected Loss

Posterior Expected Loss

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

Bayesian Decision Theory

Choose an estimator that minimizes posterior expected loss.

Easier Calculation

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

Question

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

Bayes Risk vs. Posterior Expected Loss

Theorem

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

Proof

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

Finding a Bayes Estimator

Hard Problem

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

Easy Problem

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

Punchline

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

Bayes Estimators for Common Loss Functions

Zero-one Loss

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

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

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

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

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

Derivation of Bayes Estimator for Squared Error Loss

By definition,

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

Differentiating with respect to a, we have

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

Example: Bayes Estimator for a Normal Mean

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

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

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

Hence the Bayes estimator for μ under squared error loss is

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

Minimax Analysis

Wasserman (2004)

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

Berger (1986)

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

Methods for Finding a Minimax Estimator

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

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

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 $\alpha = \beta = \sqrt{n}/2$,

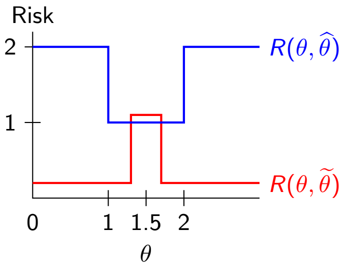
$$\widehat{p}(\mathbf{x}) = \frac{n\bar{X} + \sqrt{n}/2}{n + \sqrt{n}}$$

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:

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

Since R cannot be negative for squared error loss,

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

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

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 **y** from **x** via Linear Regression

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

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

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

Operationalizing the Bias-Variance Tradeoff Idea

Mallow's C_p

Approximate the predictive MSE of each model relative to the infeasible optimum in which $\boldsymbol{\beta}$ is known.

Notation

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

In-sample versus Out-of-sample Prediction Error

Why not compare RSS(m)?

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

From your Problem Set

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

Bias-Variance Tradeoff

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

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

Step 1: Algebra

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

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

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

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

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

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

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

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

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

Bias-Variance Tradeoff

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

Mallow's C_p

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

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

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

Notation

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

Crucial Fact

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

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

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

Bias of Plug-in Estimator

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

Putting Everything Together: Mallow's C_p

Want An Unbiased Estimator of This:

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

Previous Slide:

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

End Result:

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

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

Why is this different from the textbook formula?

Just algebra, but tedious...

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

Therefore:

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

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

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

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

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

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

where $P(m)$ is the prior model probability and $f(\mathbf{y})$ is constant across models.

Laplace (aka Saddlepoint) Approximation

Suppress model index m for simplicity.

General Case: for T large...

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

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

Use to Approximate Marginal Likelihood

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

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

Laplace Approximation to Marginal Likelihood

Suppress model index m for simplicity.

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

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

Bayesian Information Criterion

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

Take Logs and Multiply by 2

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

The BIC

Assume uniform prior over models and ignore lower order terms:

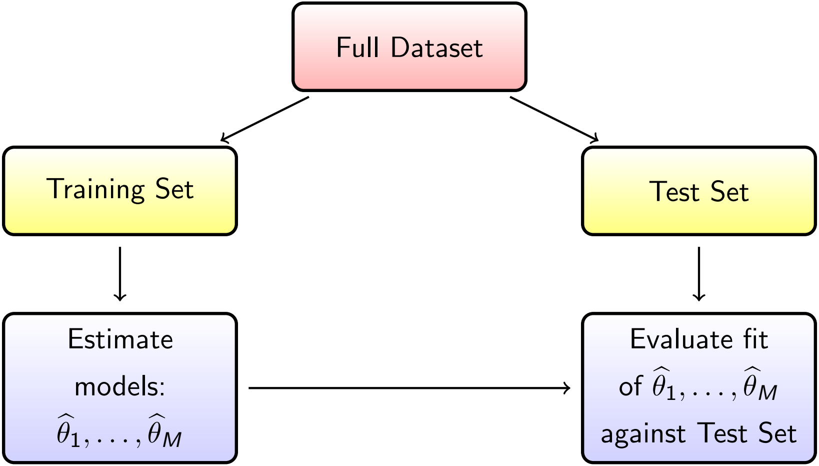
$$\text{BIC}(m) = 2\log f(\mathbf{y}|\widehat{\boldsymbol{\theta}}, m) - p_m \log(T)$$

large-sample Frequentist approx. to Bayesian marginal likelihood

Model Selection using a Hold-out Sample

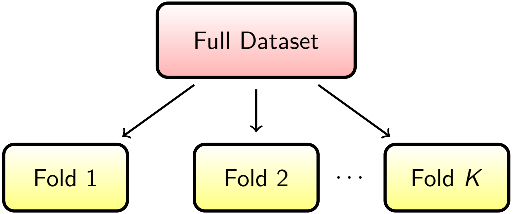
- The real problem is double use of the data: first for estimation, then for model comparison.
  - Maximized sample log-likelihood is an overly optimistic estimate of expected log-likelihood and hence KL-divergence
  - In-sample squared prediction error is an overly optimistic estimator of out-of-sample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

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

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:

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

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

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

Overview of Proof

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

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

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 a point mass at y: $\delta_y(y) = 1$, $\delta_y(y') = 0$ for $y' \neq y$.

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

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

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

Empirical CDF $\widehat{G}$

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

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

For ML estimation it turns out that:

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

Step 3

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

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

Derivation of Influence Function for MLE

I'll do this on the blackboard if we have time...

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:

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

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 $\widehat{M} = 0$ 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 $\mathrm{IC}_m = 2\ell(\theta) - d_T \times \text{length}(\theta)$.

True DGP

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

Candidate Models

M_0 assumes $\mu = 0$, M_1 does not restrict 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

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

Condition on Penalty

- Need $c_{T,k} = o_p(T)$, i.e. $c_{T,k}/T \xrightarrow{p} 0$.
- 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):

$$\begin{aligned} P\left(\widehat{M} = M_1\right) &= P\left(|\sqrt{T}\bar{Y}| \geq \sqrt{d_T}\right) = P(|Z| \geq \sqrt{d_T}) \\ &= P(Z^2 \geq d_T) = P(\chi_1^2 \geq d_T) \end{aligned}$$

- AIC: $d_T = 2$ and $P(\chi_1^2 \geq 2) \approx 0.157$.
- BIC: $d_T = \log(T)$ and $P(\chi_1^2 \geq \log T) \to 0$ 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 $\rightarrow 1$ as $T \rightarrow \infty$, 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 $\rightarrow 1$ as $T \rightarrow \infty$, the risk of the MLE
- For $\mu = 0$, risk $\rightarrow 0$, 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* functions 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) $\sup\limits_{\theta \in N_\epsilon} \left|\left| T^{-1} \sum_{t=1}^{T} \nabla_\theta f(v_t, \theta) - E[\nabla_\theta f(v_t, \theta)] \right|\right| \xrightarrow{p} 0$

Regularity Conditions for Variance of Moment Conditions

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

(ii) $\lim\limits_{T \to \infty} Var\left[\sqrt{T}\bar{g}_T(\theta_0)\right] = S$ 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: $\sqrt{T}(\widehat{\theta}_T - \theta_0) \xrightarrow{d} \mathcal{N}(0, MSM')$

$$
\begin{aligned}
M &= (G_0 W G_0)^{-1} G_0' W \\
S &= \lim_{T\to\infty} Var\left[\sqrt{T}\bar{g}_T(\theta_0)\right] \\
G_0 &= E[\nabla_{\theta'} f(v_t, \theta_0)] \\
W &= \text{plim}_{T\to\infty} W_T
\end{aligned}
$$

The J-test Statistic

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

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

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

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

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

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

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

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

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

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

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

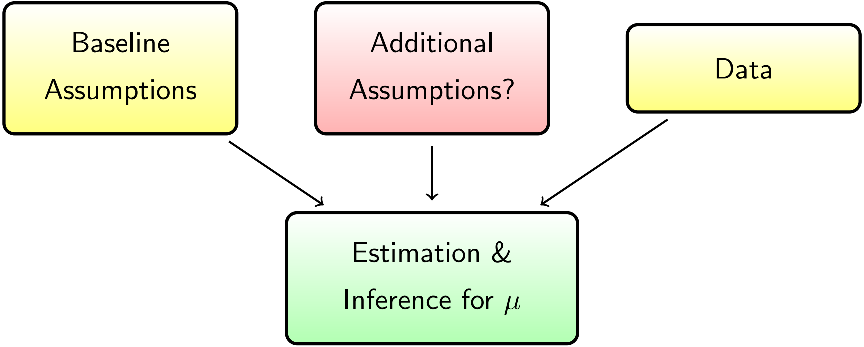
How do these examples behave?

GMM-AIC doesn't satisfy the theorem, since $\kappa_T = 2$ does not diverge as $T \to \infty$. GMM-BIC and GMM-HQ are consistent since $\lim_{T\to\infty} \log(T)/T = 0$ and $\lim_{T\to\infty} \log\big(\log(T)\big)/T = 0$.

Lecture #6 – Focused Moment Selection

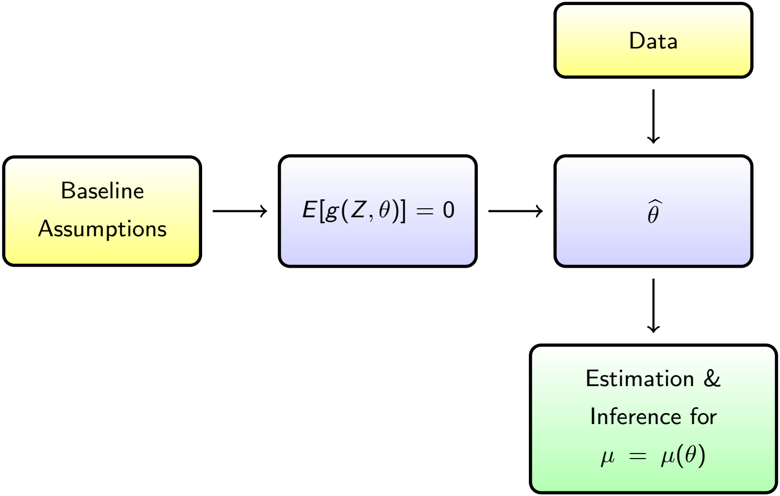
DiTraglia (2016, JoE)

Focused Moment Selection Criterion (FMSC)

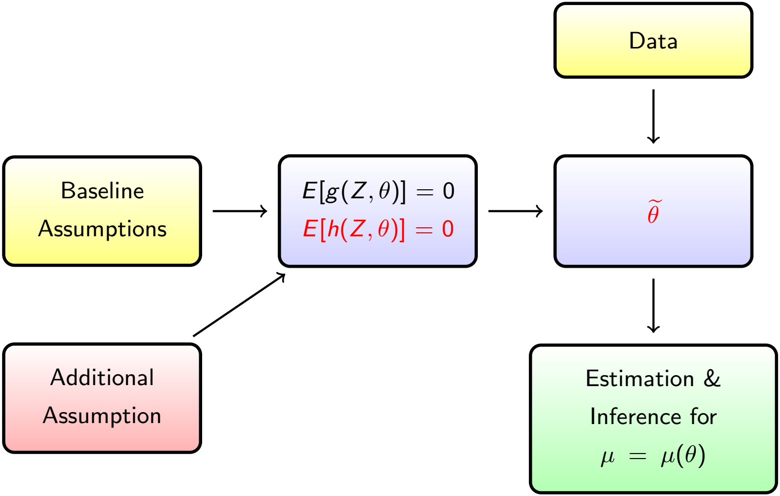


1. Choose False Assumptions on Purpose
2. Focused Choice of Assumptions
3. Local mis-specification
4. Averaging, Inference post-selection

GMM Framework



Adding Moment Conditions



Ordinary versus Two-Stage Least Squares

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

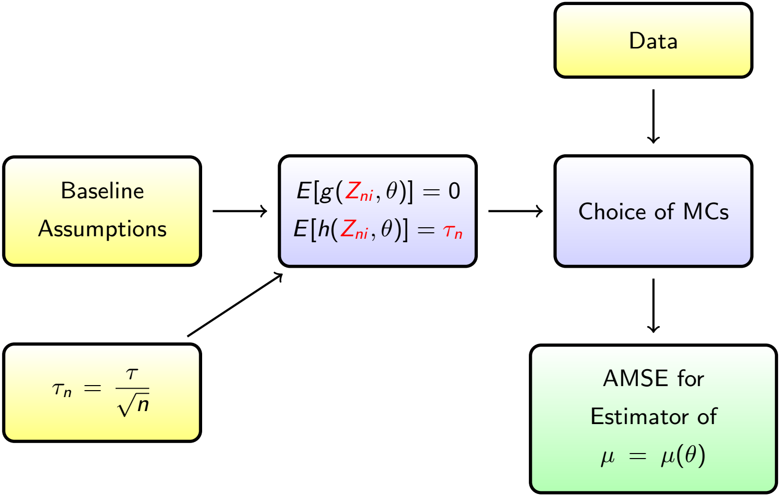
$$\begin{aligned} E[\mathbf{z}_i \epsilon_i] &= 0 \\ E[x_i \epsilon_i] &= ? \end{aligned}$$

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

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

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

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) $Z_{ni} \to_d Z_i$, 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

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

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

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

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

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

Delta Method

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

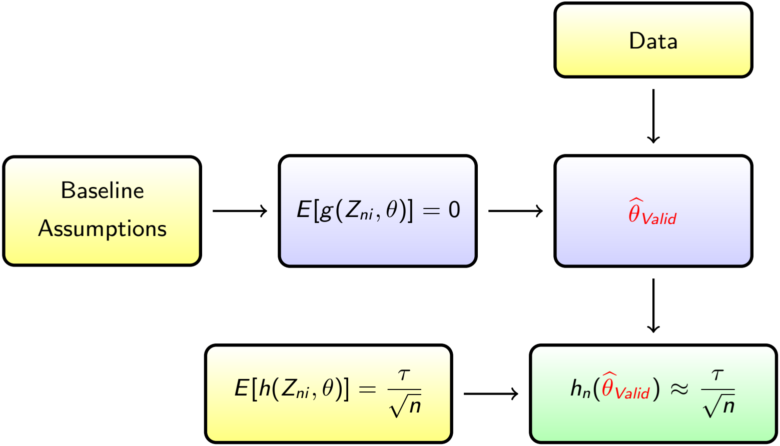
FMSC: Estimate AMSE($\widehat{\mu}_S$) and minimize over S

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

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 $\tau\tau'$

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

$$\Psi = \begin{bmatrix} -HK_v & \mathbf{I}_q \end{bmatrix}$$

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

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

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

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

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

Simulating from the Limit Experiment

Suppose τ Known, Consistent Estimators of Everything Else

1. $\texttt{for}\ j \in \{1, 2, \ldots, J\}$
   (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 $1-(\alpha+\delta)$

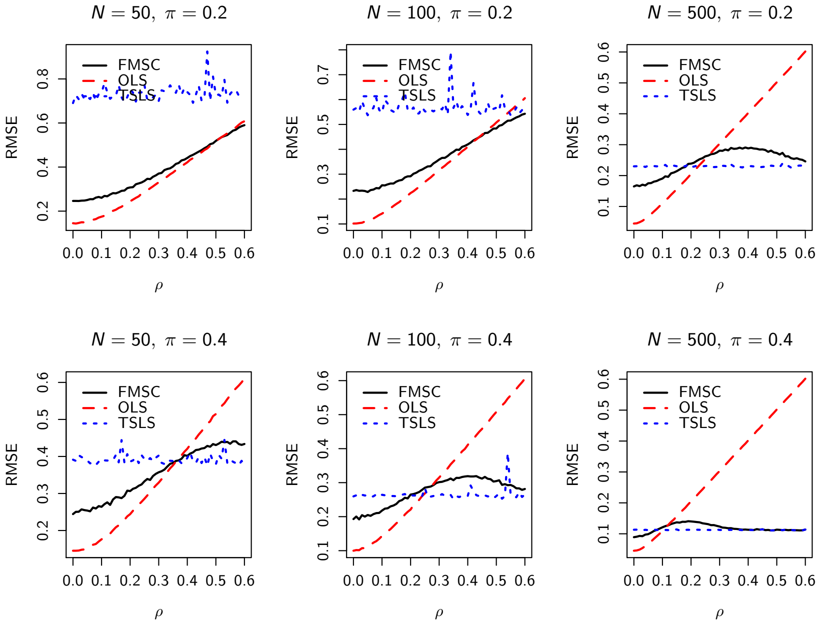
OLS versus TSLS Simulation

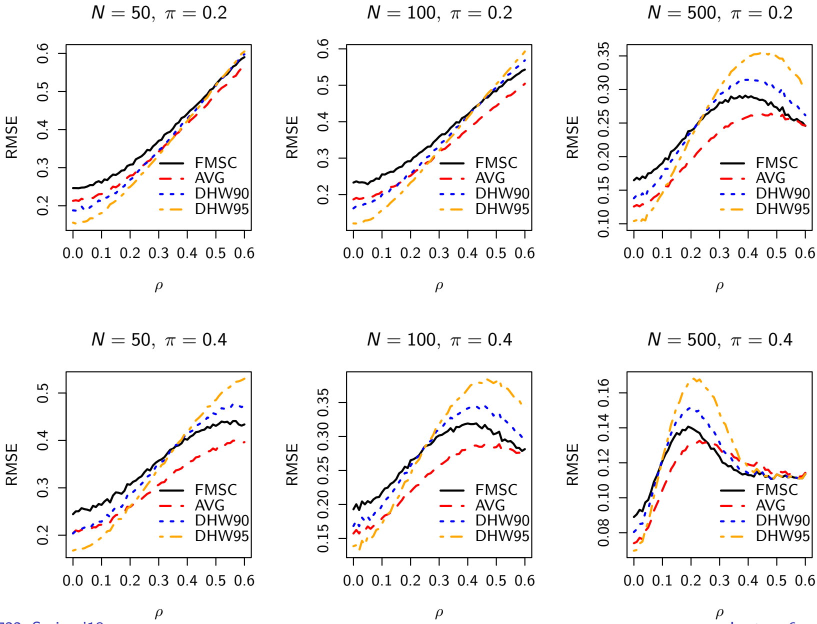
$$
\begin{aligned}
y_i &= 0.5x_i + \epsilon_i \\
x_i &= \pi(z_{1i} + z_{2i} + z_{3i}) + v_i
\end{aligned}
$$

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

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

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


N = 50, π = 0.2
N = 100, π = 0.2
N = 500, π = 0.2
N = 50, π = 0.4
N = 100, π = 0.4
N = 500, π = 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

Choosing Instrumental Variables Simulation

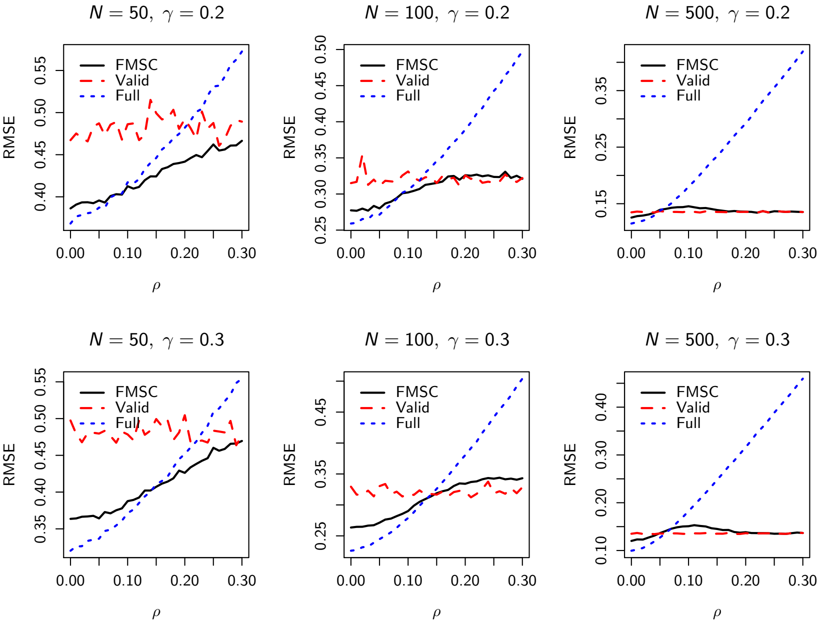
$$
\begin{aligned}
y_i &= 0.5x_i + \epsilon_i \\
x_i &= (z_{1i} + z_{2i} + z_{3i})/3 + \gamma w_i + v_i
\end{aligned}
$$

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

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

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

$$Var(x) = 1, \quad Cor(x, \epsilon) = 0.5$$



$N = 50,\ \gamma = 0.2$
$N = 100,\ \gamma = 0.2$
$N = 500,\ \gamma = 0.2$
$N = 50,\ \gamma = 0.3$
$N = 100,\ \gamma = 0.3$
$N = 500,\ \gamma = 0.3$
FMSC
Valid
Full
RMSE
ρ
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

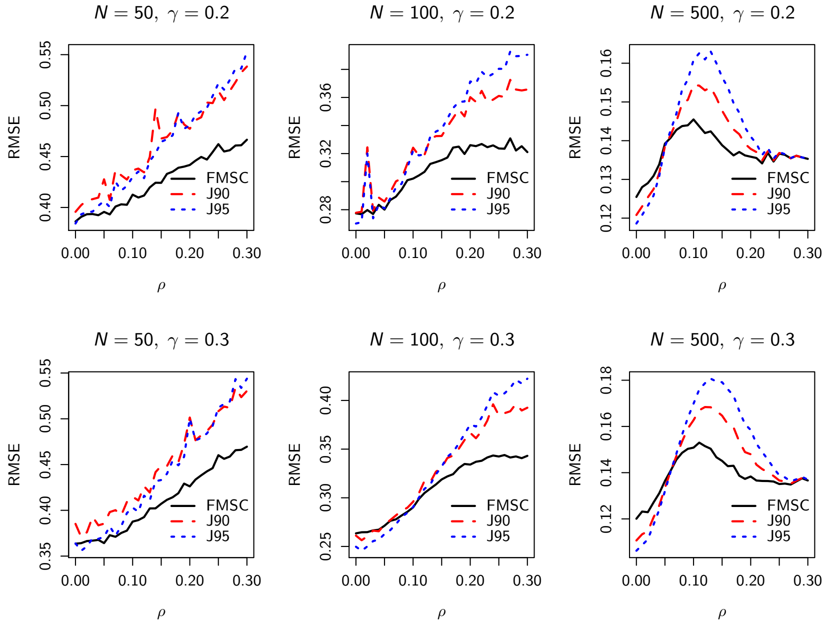
$$\text{GMM-MSC}(S) = J_n(S) - \text{Bonus}$$

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

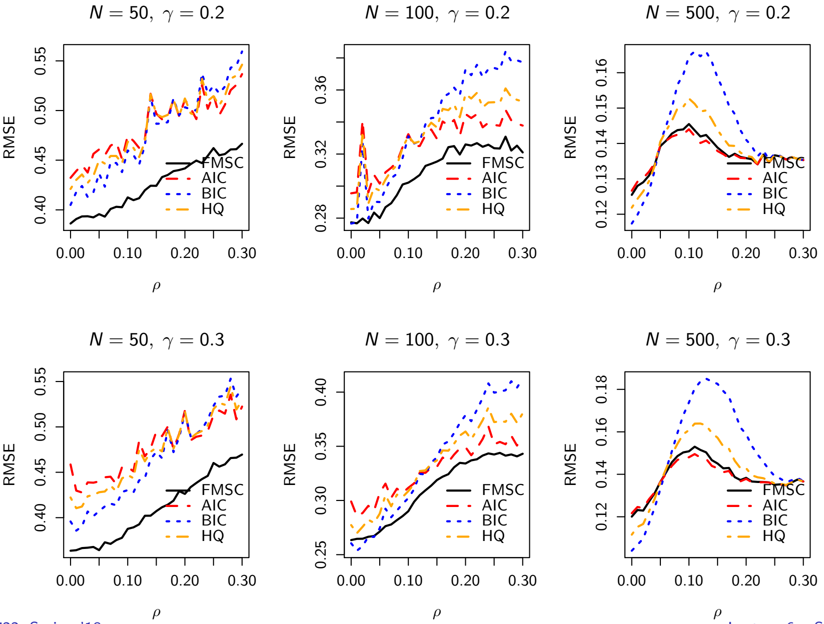
$$\text{CCIC}(S) = n \log\left[1 - R_n^2(S)\right] + \textit{Penalty}$$

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



$N = 50,\ \gamma = 0.2$
$N = 100,\ \gamma = 0.2$
$N = 500,\ \gamma = 0.2$
$N = 50,\ \gamma = 0.3$
$N = 100,\ \gamma = 0.3$
$N = 500,\ \gamma = 0.3$
RMSE
ρ
FMSC
AIC
BIC
HQ
0.00
0.10
0.20
0.30
0.40
0.45
0.50
0.55
0.28
0.32
0.36
0.12
0.13
0.14
0.15
0.16
0.25
0.30
0.35
0.40
0.18

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

Review of Principal Component Analysis (PCA)

Ridge Regression

Principal Components Regression

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

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

- $U = m \times m$ 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.

Principal Component Analysis (PCA)

Notation

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

Optimization Problem

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

First Principal Component

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

It is the direction along with $\mathbf{x}$ has maximal variation

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 $\boldsymbol{\alpha}_1'\mathbf{x}$.

jth 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 $X'X = VD^2V'$

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

Ridge Regression – OLS with an L_2 Penalty

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

- 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

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

- 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

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

since:

$$\begin{aligned} \left(\widetilde{\mathbf{y}} - \widetilde{X}\beta\right)' \left(\widetilde{\mathbf{y}} - \widetilde{X}\beta\right) &= \begin{bmatrix} (\mathbf{y} - X\beta)' & (-\sqrt{\lambda}\beta)' \end{bmatrix} \begin{bmatrix} (\mathbf{y} - X\beta) \\ -\sqrt{\lambda}\beta \end{bmatrix} \\ &= (\mathbf{y} - X\beta)'(\mathbf{y} - X\beta) + \lambda\beta'\beta \end{aligned}$$

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 $H(\lambda)$

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

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

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

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 OLS and Ridge Predictions

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

Comparing OLS and Ridge Predictions

$$\widehat{y}(\lambda) = \sum_{j=1}^{p} \left(\frac{d_j^2}{d_j^2 + \lambda} \right) \mathbf{u}_j \mathbf{u}_j' \mathbf{y}$$

- Since X is centered, $\mathbf{z}_j = d_j \mathbf{u}_j$ is the jth sample PC
- d_j^2 is proportional to the variance of the jth sample PC
- Prediction from regression of $\mathbf{y}$ on $\mathbf{z}_j$ is:

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

- Ridge equivalent to regressing y on sample PCs of X but shrinking predictions to zero: higher variance PCs are shrunk less.
- OLS doesn't shrink.

Principal Components Regression (PCR)

Instead of "smooth weights" as in Ridge, truncate the PCs:

1. Calculate SVD $X = UDV'$ of centered data matrix X
2. Construct the sample principal components: $\mathbf{z}_i = d_j \mathbf{u}_j$.
3. Throw away all but first k principal components, where $k < p$.
4. Regress $\mathbf{y}$ on $\mathbf{z_1}, \ldots, \mathbf{z}_k$.

PCR versus Ridge

- PCR is a much less smooth version of Ridge
- Conventional wisdom is that PCR will perform worse since it shrinks low variance directions too much and doesn't shrink high variance directions at all.
- However, Dhillon et al. (2013) show that the MSE risk of PCR is always within a constant factor of that of Ridge Regression while there are situations in which Ridge can be arbitrarily worse than PCR in terms of MSE.
- In practice, which is better depends on the DGP

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

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

LASSO – L_1 Penalty

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

Other Ways of Thinking about LASSO

Constrained Optimization

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

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

Bayesian Posterior Mode

Ignoring the intercept, LASSO is the posterior model 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

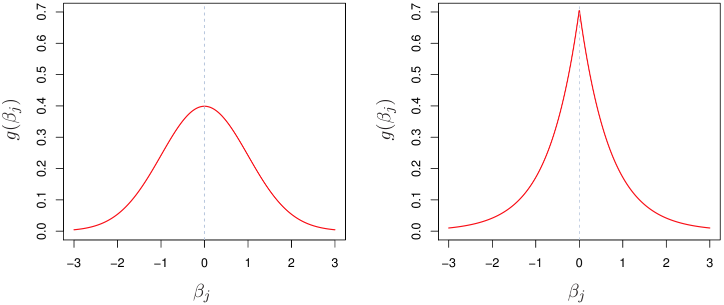


Figure: Ridge, at left, puts a normal prior on β while LASSO, at right, uses a Laplace prior, which has fatter tails and a taller peak at zero.

Comparing LASSO and Ridge – Constrained OLS

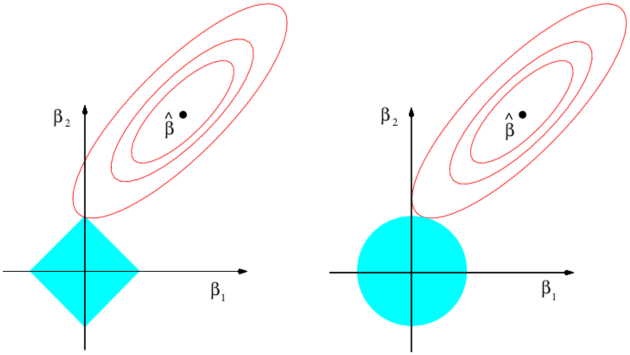


Figure: $\widehat{\beta}$ denotes the MLE and the ellipses are the contours of the likelihood. LASSO, at left, and Ridge, at right, both shrink β away from the MLE towards zero. Because of its diamond-shaped constraint set, however, LASSO favors a sparse solution while Ridge does not

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

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

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

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

LASSO when $X'X = I_p$

Preceding Slide

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

Key Simplification

Equivalent to solving j independent optimization problems:

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

- 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:

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

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

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

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 $X'X = I_p$

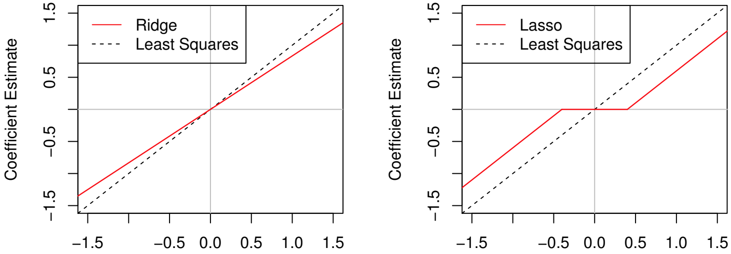


Figure: Horizontal axis in each plot is MLE

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

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

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

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

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

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

$\quad\quad c_j \leftarrow 2\sum_{i=1}^{n} x_{ij}(y_i - \mathbf{x}_i'\beta + \beta_j x_{ij})$

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

$\quad$ **end**

until $\sum_{j=1}^{p} |\beta_j^{prev} - \beta_j| < \varepsilon$;