

Econ 722 – Advanced Econometrics IV, Part II

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Lecture #1 – AIC-type Information Criteria

Kullback-Leibler Divergence

Bias of Maximized Sample Log-Likelihood

Review of Asymptotics for Mis-specified MLE

Deriving AIC and TIC

Corrected AIC (AIC_c)

Kullback-Leibler (KL) Divergence

Motivation

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

Definition

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

Properties

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

KL Divergence and Mis-specified MLE

Pseudo-true Parameter Value θ_0

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

What if f_{θ} is correctly specified?

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

Goal: Compare Mis-specified Models

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

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

How to Estimate Expected Log Likelihood?

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

Unbiased but Infeasible

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

Biased but Feasible

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

Intuition for the Bias

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

What to do about this bias?

1. General-purpose asymptotic approximation of “degree of over-optimism” of maximized sample log-likelihood.
 - ▶ Takeuchi’s Information Criterion (TIC)
 - ▶ Akaike’s Information Criterion (AIC)
2. Problem-specific finite sample approach, assuming $g \in f_\theta$.
 - ▶ Corrected AIC (AIC_c) of Hurvich and Tsai (1989)

Tradeoffs

TIC is most general and makes weakest assumptions, but requires very large T to work well. AIC is a good approximation to TIC that requires less data. Both AIC and TIC perform poorly when T is small relative to the number of parameters, hence AIC_c .

Recall: Asymptotics for Mis-specified ML Estimation

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

Fundamental Expansion

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

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

Central Limit Theorem

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

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

Information Matrix Equality

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

Bias Relative to Infeasible Plug-in Estimator

Definition of Bias Term B

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

Question to Answer

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

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

Derivation of AIC/TIC

Step 1: Taylor Expansion

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

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

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

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

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

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

Derivation of AIC/TIC Continued...

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

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

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

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

Final Result:

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

TIC and AIC

Takeuchi's Information Criterion

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

Akaike's Information Criterion

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

Contrasting AIC and TIC

Technically, AIC requires that all models under consideration are at least correctly specified while TIC doesn't. But $J^{-1}K$ is hard to estimate, and if a model is badly mis-specified, $\ell(\hat{\theta})$ dominates.

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

Idea Behind AIC_c

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

Assumption: True DGP

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

Can Show That

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

Where f is a normal regression model with parameters (β_1, σ_1^2) that might not be the true parameters.

But how can we use this?

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

1. Would need to know (β_1, σ_1^2) for **candidate model**.
 - ▶ Easy: just use MLE $(\hat{\beta}_1, \hat{\sigma}_1^2)$
2. Would need to know (β_0, σ_0^2) for **true model**.
 - ▶ Very hard! The whole problem is that we don't know these!

Hurvich & Tsai (1989) Assume:

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

Deriving the Corrected AIC

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

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

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

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

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

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

a finite-sample unbiased estimator of KL for model comparison

Lecture #2 – More on “Classical” Model Selection

Mallow's C_p

Bayesian Model Comparison

Laplace Approximation

Bayesian Information Criterion (BIC)

Motivation: Predict \mathbf{y} from \mathbf{x} via Linear Regression

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

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

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

Operationalizing the Bias-Variance Tradeoff Idea

Mallow's C_p

Approximate the predictive MSE of each model relative to the infeasible optimum in which β is known.

Notation

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

In-sample versus Out-of-sample Prediction Error

Why not compare $RSS(m)$?

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

From your Problem Set

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

Bias-Variance Tradeoff

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

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

Step 1: Algebra

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

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

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

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

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

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

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

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

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

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

Bias-Variance Tradeoff

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

Mallow's C_p

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

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

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

Notation

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

Crucial Fact

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

Step 4: Algebra using the preceding fact

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

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

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

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

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

Bias of Plug-in Estimator

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

Putting Everything Together: Mallows's C_p

Want An Unbiased Estimator of This:

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

Previous Slide:

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

End Result:

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

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

Why is this different from the textbook formula?

Just algebra, but tedious. . .

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

Therefore:

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

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

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

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

Bayesian Model Comparison: Marginal Likelihoods

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

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

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

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

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

Laplace (aka Saddlepoint) Approximation

Suppress model index m for simplicity.

General Case: for T large...

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

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

Use to Approximate Marginal Likelihood

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

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

Laplace Approximation to Marginal Likelihood

Suppress model index m for simplicity.

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

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

Bayesian Information Criterion

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

Take Logs and Multiply by 2

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

The BIC

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

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

large-sample Frequentist approx. to Bayesian marginal likelihood

Lecture #3 – Cross-Validation

Model selection via a Hold-out Sample

K-fold Cross-validation

Asymptotic Equivalence Between LOO-CV and TIC

Influence Functions

Model Selection using a Hold-out Sample

- ▶ The real problem is **double** use of the data: first for estimation, then for model comparison.
 - ▶ Maximized sample log-likelihood is an overly optimistic estimate of expected log-likelihood and hence KL-divergence
 - ▶ In-sample squared prediction error is an overly optimistic estimator of out-of-sample squared prediction error
- ▶ AIC/TIC, AIC_c , BIC, C_p **penalize** sample log-likelihood or RSS to compensate.
- ▶ Another idea: **don't re-use the same data!**

Hold-out Sample: Partition the Full Dataset



Unfortunately this is extremely wasteful of data...

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



Step 1

Randomly partition full dataset into K folds of approx. equal size.

Step 2

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

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

Step 2

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

Step 3

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

Step 4

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

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

Step 4

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

Step 5

Define $CV_K = \frac{1}{T} \sum_{t=1}^T L(y_t, \hat{y}_t^{-k(t)})$ where L is a loss function.

Step 5

Repeat for each model & choose m to minimize $CV_K(m)$.

CV uses each observation for parameter estimation and model evaluation but never at the same time!

Cross-Validation (CV): Some Details

Which Loss Function?

- ▶ For regression squared error loss makes sense
- ▶ For classification (discrete prediction) could use zero-one loss.
- ▶ Can also use log-likelihood/KL-divergence as a loss function. . .

How Many Folds?

- ▶ One extreme: $K = 2$. Closest to Training/Test idea.
- ▶ Other extreme: $K = T$ **Leave-one-out** CV (LOO-CV).
- ▶ Computationally expensive model \Rightarrow may prefer fewer folds.
- ▶ If your model is a linear smoother there's a computational trick that makes LOO-CV extremely fast. (Problem Set)
- ▶ Asymptotic properties are related to K . . .

Relationship between LOO-CV and TIC

Theorem

LOO-CV using KL-divergence as the loss function is asymptotically equivalent to TIC but doesn't require us to estimate the Hessian and variance of the score.

Large-sample Equivalence of LOO-CV and TIC

Notation and Assumptions

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

Log-likelihood as “Loss”

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

Overview of the Proof

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

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

Crucial point: the first-order term is not zero in this case. (Why?)

Overview of Proof

From expansion on previous slide, we simply need to show that:

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

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

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

Overview of Proof

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

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

So it suffices to show that

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

Digression: Functionals and Influence Functions

(Statistical) Functional

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

Example: ML Estimation

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

Influence Function

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

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

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

Back to the Proof...

Step 1

The influence function for ML estimation turns out to be

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

Step 2

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

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

Step 3

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

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

Lecture #4 – Asymptotic Properties

Overview

Weak Consistency

Consistency

Efficiency

AIC versus BIC in a Simple Example

Overview

- ▶ What happens as $T \rightarrow \infty$?
- ▶ Consistency: choose “best” model wpa 1
- ▶ Efficiency: procedure with good risk properties
- ▶ Can't have both at once.
- ▶ Large, fairly technical literature: only a brief overview today.
- ▶ More details: Sin and White (1992, 1996), Pötscher (1991), Leeb & Pötscher (2005), Yang (2005) and Yang (2007).

Penalizing the Likelihood

Examples we've seen:

$$TIC = 2\ell_T(\hat{\theta}) - \text{trace} \left\{ \hat{J}^{-1} \hat{K} \right\}$$

$$AIC = 2\ell_T(\hat{\theta}) - 2 \text{ length}(\theta)$$

$$BIC = 2\ell_T(\hat{\theta}) - \log(T) \text{ length}(\theta)$$

Generic penalty $c_{T,k}$

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

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

Weak Consistency: Suppose M_{k_0} Uniquely Minimizes KL

Assumption

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

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 $T^{-1}c_{T,k} \xrightarrow{P} 0$.

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

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

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

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

Sufficient Conditions

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

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

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

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

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

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:

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

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

Efficiency

- ▶ Roughly speaking, a model selection criterion is called efficient if it performs “nearly as well” as the theoretical optimum relative to some loss function.
- ▶ More broadly, an efficient/conservative criterion is one that has “good risk properties.”
- ▶ We don’t have time to go into detail, so we’ll look at a particular example. . .

Consistency versus Efficiency in a Simple Example

Information Criteria

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

True DGP

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

Candidate Models

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

$$IC_0 = 2 \max_{\mu} \{\ell(\mu) : M_0\}$$

$$IC_1 = 2 \max_{\mu} \{\ell(\mu) : M_1\} - d_T$$

Log-Likelihood Function

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

$$\begin{aligned}\ell_T(\mu) &= \sum_{t=1}^T \log \left(\frac{1}{2\pi} \exp \left\{ -\frac{1}{2} (Y_t - \mu)^2 \right\} \right) \\&= -\frac{T}{2} \log(2\pi) - \frac{1}{2} \sum_{t=1}^T (Y_t - \mu)^2 \\&= -\frac{T}{2} \log(2\pi) - \frac{T}{2} \hat{\sigma}^2 - \frac{T}{2} (\bar{Y} - \mu)^2 \\&= \text{Constant} - \frac{T}{2} (\bar{Y} - \mu)^2\end{aligned}$$

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

$$\begin{aligned} T\hat{\sigma}^2 &= \sum_{t=1}^T (Y_t - \bar{Y})^2 = \sum_{t=1}^T (Y_t - \mu + \mu - \bar{Y})^2 = \sum_{t=1}^T [(Y_t - \mu) - (\bar{Y} - \mu)]^2 \\ &= \sum_{t=1}^T (Y_t - \mu)^2 - \sum_{t=1}^T 2(Y_t - \mu)(\bar{Y} - \mu) + \sum_{t=1}^T (\bar{Y} - \mu)^2 \\ &= \left[\sum_{t=1}^T (Y_t - \mu)^2 \right] - 2(\bar{Y} - \mu) \left(\sum_{t=1}^T Y_t - \sum_{t=1}^T \mu \right) + T(\bar{Y} - \mu)^2 \\ &= \left[\sum_{t=1}^T (Y_t - \mu)^2 \right] - 2(\bar{Y} - \mu)(T\bar{Y} - T\mu) + T(\bar{Y} - \mu)^2 \\ &= \left[\sum_{t=1}^T (Y_t - \mu)^2 \right] - 2T(\bar{Y} - \mu)^2 + T(\bar{Y} - \mu)^2 \\ &= \left[\sum_{t=1}^T (Y_t - \mu)^2 \right] - T(\bar{Y} - \mu)^2 \end{aligned}$$

The Selected Model \hat{M}

Information Criteria

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

$$IC_0 = 2 \max_{\mu} \{\ell(\mu) : M_0\} = 2 \times \text{Constant} - T\bar{Y}^2$$

$$IC_1 = 2 \max_{\mu} \{\ell(\mu) : M_1\} - d_T = 2 \times \text{Constant} - d_T$$

Difference of Criteria

$$IC_1 - IC_0 = T\bar{Y}^2 - d_T$$

Selected Model

$$\hat{M} = \begin{cases} M_1, & |\sqrt{T}\bar{Y}| \geq \sqrt{d_T} \\ M_0, & |\sqrt{T}\bar{Y}| < \sqrt{d_T} \end{cases}$$

Case I: $\mu \neq 0$

Apply theory from earlier in lecture...

KL-Divergence of M_1

M_1 is the true DGP with minimized KL-divergence equal to zero.

KL-Divergence of M_0

- ▶ Truth: $g(y) = (2\pi)^{-1/2} \exp \{-(y - \mu)^2/2\}$
- ▶ M_0 : $f(y) = (2\pi)^{-1/2} \exp \{-y^2/2\}$
- ▶ Hence: $\log g(y) - \log f(y) = -\frac{1}{2}(y - \mu)^2 + \frac{1}{2}y^2 = \mu(y - \frac{\mu}{2})$

$$\begin{aligned} \text{KL}(g; M_0) &= \int_{\mathbb{R}} \mu(y - \mu/2)(2\pi)^{-1/2} \exp \{(y - \mu)^2/2\} dy \\ &= \mu(\mu - \mu/2) = \mu^2/2 \end{aligned}$$

Verifying Weak Consistency: $\mu \neq 0$

Condition on KL-Divergence

$$\liminf_{T \rightarrow \infty} \frac{1}{T} \sum_{t=1}^T \{KL(g; M_0) - KL(g; M_1)\} = \liminf_{n \rightarrow \infty} \frac{1}{T} \sum_{t=1}^T \left(\frac{\mu^2}{2} - 0 \right) > 0$$

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 $T \rightarrow \infty$.

Case II: $\mu = 0$

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 $\mathbb{P}(c_{T,k} - c_{T,0}) \rightarrow \infty$
- ▶ BIC satisfies this but AIC doesn't.

Finite-Sample Selection Probabilities: AIC

AIC Sets $d_T = 2$

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

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

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

Finite-Sample Selection Probabilities: BIC

BIC sets $d_T = \log(T)$

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

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

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

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):

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

- ▶ AIC: $d_T = 2$ and $P(\chi_1^2 \geq 2) \approx 0.157$.
- ▶ BIC: $d_T = \log(T)$ and $P(\chi_1^2 \geq \log T) \rightarrow 0$ as $T \rightarrow \infty$.

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

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

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 since Var. of well-behaved estimator $= O(1/T)$

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

Simplifying the MSE Risk Function

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

Let $X = \mathbf{1}\{A\}$ where $A = \left\{|\sqrt{T}\mu + Z| \geq \sqrt{dT}\right\}$

$$\begin{aligned}R_T(\mu) &= \mathbb{E} \left[\left(\sqrt{T}\hat{\mu} - \sqrt{T}\mu \right)^2 \right] \\&= \mathbb{E} \left\{ \left[\left(\sqrt{T}\mu + Z \right) X - \sqrt{T}\mu \right]^2 \right\} \\&= \mathbb{P}(A) \mathbb{E} \left\{ \left[\left(\sqrt{T}\mu + Z \right) - \sqrt{T}\mu \right]^2 \middle| X = 1 \right\} + [1 - \mathbb{P}(A)] \left(\sqrt{T}\mu \right)^2 \\&= \mathbb{P}(A) \mathbb{E} \left[Z^2 | X = 1 \right] + [1 - \mathbb{P}(A)] T\mu^2\end{aligned}$$

So we need to calculate $\mathbb{P}(A) \mathbb{E}[Z^2 | X = 1]$ and $\mathbb{P}(A)$.

Calculating $\mathbb{P}(A)$

Define $a = (-\sqrt{d_T} - \sqrt{T}\mu)$ and $b = (\sqrt{d_T} - \sqrt{T}\mu)$

$$\begin{aligned}\mathbb{P}(A) &= \mathbb{P}\left(|\sqrt{T}\mu + Z| \geq \sqrt{d_T}\right) \\&= \mathbb{P}\left(\sqrt{T}\mu + Z \geq \sqrt{d_T}\right) + \mathbb{P}\left(\sqrt{T}\mu + Z \leq -\sqrt{d_T}\right) \\&= \mathbb{P}(Z \geq b) + \mathbb{P}(Z \leq a) \\&= 1 - \Phi(b) + \Phi(a)\end{aligned}$$

And hence:

$$1 - \mathbb{P}(A) = \Phi(b) - \Phi(a)$$

Calculating $\mathbb{P}(A) \mathbb{E}[Z^2|X = 1]$ – Step 1

Conditional Density of $Z|X = 1$

$$f(z|x = 1) = \frac{\mathbf{1}(A)\varphi(z)}{\mathbb{P}(A)} \quad \text{where } \varphi \text{ is the } N(0, 1) \text{ density}$$

Therefore:

$$\begin{aligned}\mathbb{P}(A) \mathbb{E}[Z^2|X = 1] &= \mathbb{P}(A) \int_{\mathbb{R}} z^2 \left[\frac{\mathbf{1}(A)\varphi(z)}{\mathbb{P}(A)} \right] dz \\ &= \int_{-\infty}^a z^2 \varphi(z) dz + \int_b^{\infty} z^2 \varphi(z) dz\end{aligned}$$

Calculating $\mathbb{P}(A) \mathbb{E}[Z^2|X = 1]$ – Step 2

Unconditional Expectation: $\mathbb{E}[Z^2]$

$$1 = \mathbb{E}[Z^2] = \int_{-\infty}^a z^2 \varphi(z) \, dz + \int_a^b z^2 \varphi(z) \, dz + \int_b^{\infty} z^2 \varphi(z) \, dz$$

Therefore:

$$\begin{aligned} \mathbb{P}(A) \mathbb{E}[Z^2|X = 1] &= \int_{-\infty}^a z^2 \varphi(z) \, dz + \int_b^{\infty} z^2 \varphi(z) \, dz \\ &= 1 - \int_a^b z^2 \varphi(z) \, dz \end{aligned}$$

Calculating $\mathbb{P}(A) \mathbb{E}[Z^2|X = 1]$ – Step 3

Integration By Parts

Take $u = -z$ and $dv = -z \exp\{-z^2/2\}$ since

$$\frac{d}{dz} (\exp\{-z^2/2\}) = -z \exp\{-z^2/2\}$$

Thus, $v = \exp\{-z^2/2\}$, $du = -1$ and

$$\begin{aligned} \int_a^b z^2 \phi(z) dz &= (2\pi)^{-1/2} \int_a^b z^2 \exp\{-z^2/2\} dz \\ &= (2\pi)^{-1/2} \left[-z \exp\{-z^2/2\} \Big|_a^b + \int_a^b \exp\left\{-\frac{z^2}{2}\right\} dz \right] \\ &= a\phi(a) - b\phi(b) + \Phi(b) - \Phi(a) \end{aligned}$$

The Simplified MSE Risk Function

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

where

$$a = -\sqrt{d_T} - \sqrt{T}\mu$$

$$b = \sqrt{d_T} - \sqrt{T}\mu$$

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

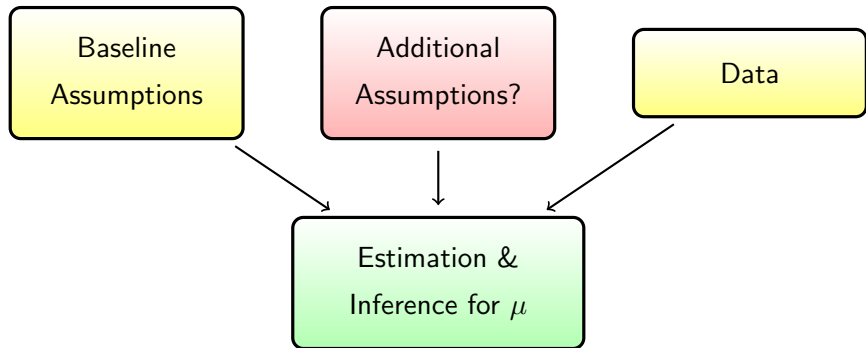
Punchline: Risk of the Post-Selection Estimator

- ▶ AIC: bounded worst-case risk
- ▶ BIC: low risk in a neighborhood of $\mu = 0$ in exchange for **unbounded** worst-case risk as sample size grows
- ▶ General phenomenon: consistency and efficiency are mutually exclusive: consistent criteria have unbounded worst-case risk.
- ▶ For more details, see Yang (2007, ET)

Lecture #7 – Focused Moment Selection

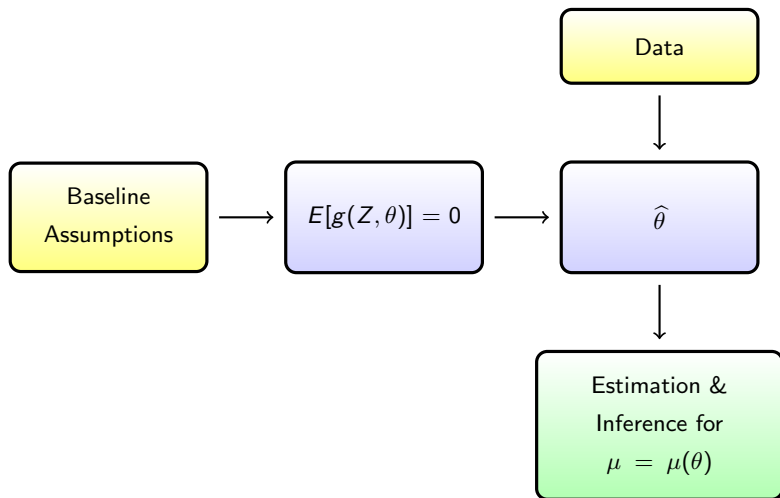
DiTraglia (2016, JoE)

Focused Moment Selection Criterion (FMSC)

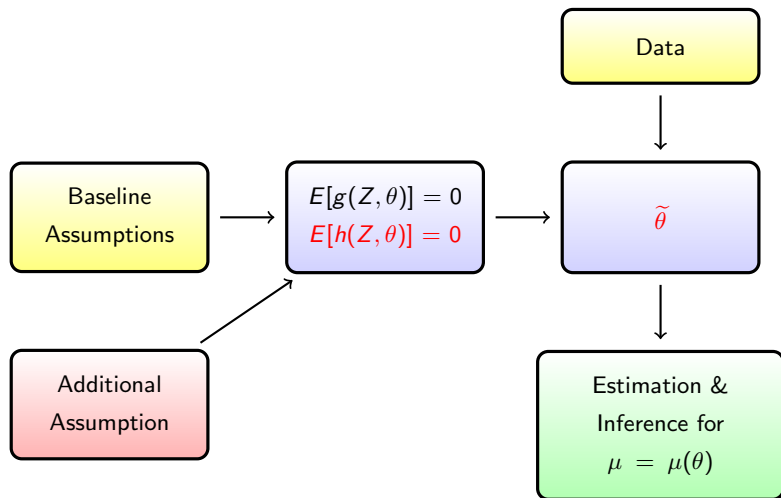


1. Choose False Assumptions on Purpose
2. Focused Choice of Assumptions
3. Local mis-specification
4. Averaging, Inference post-selection

GMM Framework



Adding Moment Conditions



Ordinary versus Two-Stage Least Squares

$$y_i = \beta x_i + \epsilon_i$$

$$x_i = \mathbf{z}_i' \boldsymbol{\pi} + v_i$$

$$E[\mathbf{z}_i \epsilon_i] = 0$$

$$E[x_i \epsilon_i] = ?$$

Choosing Instrumental Variables

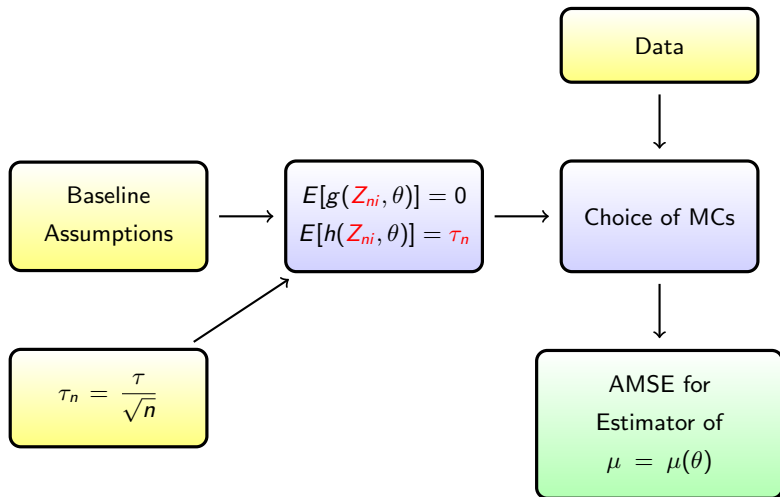
$$y_i = \beta x_i + \epsilon_i$$

$$x_i = \Pi'_1 \mathbf{z}_i^{(1)} + \Pi'_2 \mathbf{z}_i^{(2)} + v_i$$

$$E[\mathbf{z}_i^{(1)} \epsilon_i] = 0$$

$$E[\mathbf{z}_i^{(2)} \epsilon_i] = ?$$

FMSC Asymptotics – Local Mis-Specification



Local Mis-Specification for OLS versus TSLS

$$y_i = \beta x_i + \epsilon_i$$

$$x_i = \mathbf{z}_i' \boldsymbol{\pi} + v_i$$

$$E[\mathbf{z}_i \epsilon_i] = 0$$

$$E[x_i \epsilon_i] = \tau / \sqrt{n}$$

Local Mis-Specification for Choosing IVs

$$\begin{aligned}y_i &= \beta x_i + \epsilon_i \\x_i &= \Pi'_1 \mathbf{z}_i^{(1)} + \Pi'_2 \mathbf{z}_i^{(2)} + v_i\end{aligned}$$

$$E[\mathbf{z}_i^{(1)} \epsilon_i] = 0$$

$$E[\mathbf{z}_i^{(1)} v_i] = \tau / \sqrt{n}$$

Local Mis-Specification

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

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

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

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

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

Shorthand: Write Z for Z_i

Candidate GMM Estimator

$$\hat{\theta}_S = \arg \min_{\theta \in \Theta} [\Xi_S f_n(\theta)]' \widetilde{W}_S [\Xi_S f_n(\theta)]$$

Ξ_S = Selection Matrix (ones and zeros)

\widetilde{W}_S = Weight Matrix (p.s.d.)

$$f_n(\theta) = \begin{bmatrix} g_n(\theta) \\ h_n(\theta) \end{bmatrix} = \begin{bmatrix} n^{-1} \sum_{i=1}^n g(Z_{ni}, \theta) \\ n^{-1} \sum_{i=1}^n h(Z_{ni}, \theta) \end{bmatrix}$$

Notation: Limit Quantities

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

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

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

Local Mis-Specification + Standard Regularity Conditions

Every candidate estimator is consistent for θ_0 and

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

$$K_S = [F_S' W_S F_S]^{-1} F_S' W_S$$

$$M = (M_g', M_h')'$$

$$M \sim N(0, \Omega)$$

Scalar Target Parameter μ

$$\mu = \mu(\theta) \quad \text{Z-a.s. continuous function}$$

$$\mu_0 = \mu(\theta_0) \quad \text{true value}$$

$$\hat{\mu} = \mu(\hat{\theta}_S) \quad \text{estimator}$$

Delta Method

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

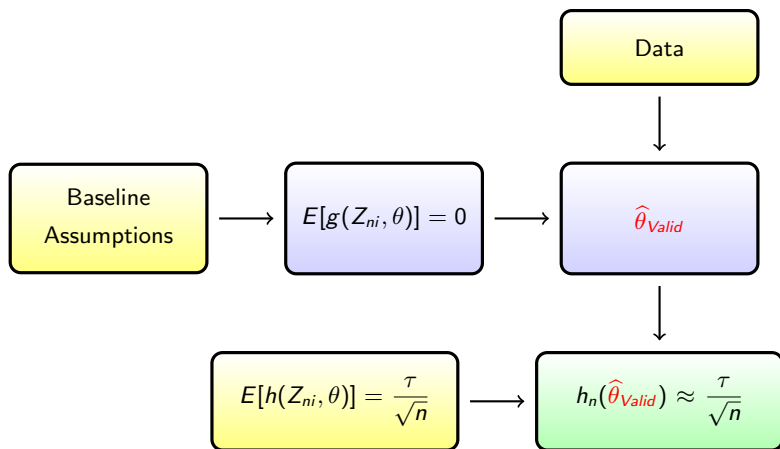
FMSC: Estimate $\text{AMSE}(\hat{\mu}_S)$ and minimize over S

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

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 $\tau\tau'$

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

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

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

FMSC: Asymptotically Unbiased Estimator of AMSE

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

$$\hat{B} = \hat{\tau} \hat{\tau}' - \hat{\psi} \hat{\Omega} \hat{\psi}'$$

Choose S to minimize $\text{FMSC}_n(S)$ over the set of candidates \mathcal{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 $\alpha \approx 0.16$

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

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

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

Conservative criterion: random even in the limit.

Moment Average Estimators

$$\hat{\mu} = \sum_{S \in \mathcal{S}} \hat{w}_S \hat{\mu}_S$$

Additional Notation

$\hat{\mu}$ Moment-average Estimator

$\hat{\mu}_S$ Estimator of target parameter under moment set S

\hat{w}_S Data-dependent weight function

\mathcal{S} Collection of moment sets under consideration

Examples of Moment-Averaging Weights

Post-Moment Selection Weights

$$\hat{\omega}_S = \mathbf{1} \{ \text{MSC}_n(S) = \min_{S' \in \mathcal{S}} \text{MSC}_n(S') \}$$

Exponential Weights

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

Minimum-AMSE Weights...

Minimum AMSE-Averaging Estimator: OLS vs. TSLS

$$\tilde{\beta}(\omega) = \omega \hat{\beta}_{OLS} + (1 - \omega) \tilde{\beta}_{TSLS}$$

Under homoskedasticity:

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

Estimate by:

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

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

Limit Distribution of Moment-Average Estimators

$$\hat{\mu} = \sum_{S \in \mathcal{S}} \hat{\omega}_S \hat{\mu}_S$$

- (i) $\sum_{S \in \mathcal{S}} \hat{\omega}_S = 1$ a.s.
- (ii) $\hat{\omega}(S) \rightarrow_d \varphi_S(\tau, M)$ a.s.-continuous function of τ , M and consistently-estimable constants only

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

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

Simulating from the Limit Experiment

Suppose τ Known, Consistent Estimators of Everything Else

- for $j \in \{1, 2, \dots, J\}$
 - $M_j \stackrel{iid}{\sim} N_{p+q} \left(0, \hat{\Omega} \right)$
 - $\Lambda_j(\tau) = -\nabla_{\theta} \mu(\hat{\theta})' \left[\sum_{s \in \mathcal{S}} \hat{\varphi}_s(M_j + \tau) \hat{K}_s \Xi_s \right] (M_j + \tau)$
- Using $\{\Lambda_j(\tau)\}_{j=1}^J$ calculate $\hat{a}(\tau)$, $\hat{b}(\tau)$ such that
$$P \left[\hat{a}(\tau) \leq \Lambda(\tau) \leq \hat{b}(\tau) \right] = 1 - \alpha$$
- $P \left[\hat{\mu} - \hat{b}(\tau)/\sqrt{n} \leq \mu_0 \leq \hat{\mu} - \hat{a}(\tau)/\sqrt{n} \right] \approx 1 - \alpha$

Two-step Procedure for Conservative Intervals

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

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

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

OLS versus TSLS Simulation

$$y_i = 0.5x_i + \epsilon_i$$

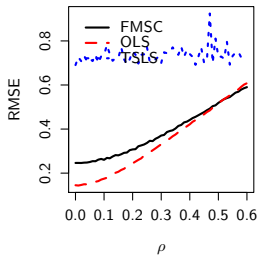
$$x_i = \pi(z_{1i} + z_{2i} + z_{3i}) + v_i$$

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

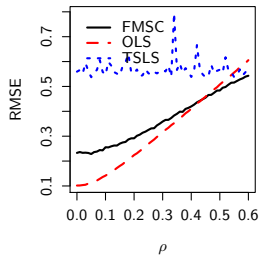
$$\mathcal{S} = \begin{bmatrix} 1 & \rho & 0 & 0 & 0 \\ \rho & 1 - \pi^2 & 0 & 0 & 0 \\ 0 & 0 & 1/3 & 0 & 0 \\ 0 & 0 & 0 & 1/3 & 0 \\ 0 & 0 & 0 & 0 & 1/3 \end{bmatrix}$$

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

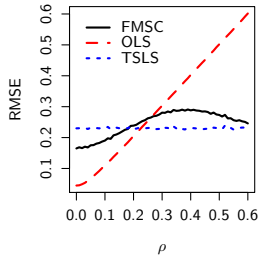
$N = 50, \pi = 0.2$



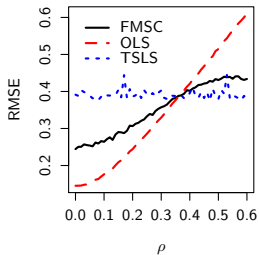
$N = 100, \pi = 0.2$



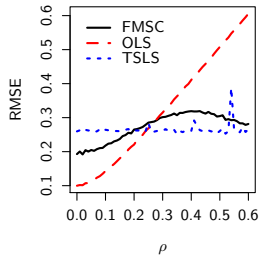
$N = 500, \pi = 0.2$



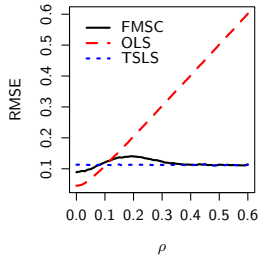
$N = 50, \pi = 0.4$



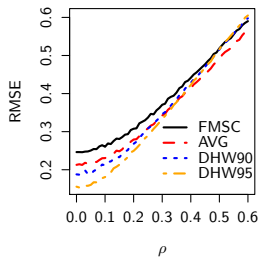
$N = 100, \pi = 0.4$



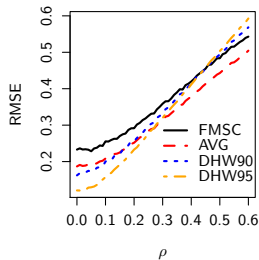
$N = 500, \pi = 0.4$



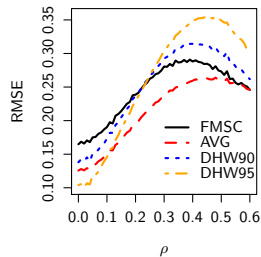
$N = 50, \pi = 0.2$



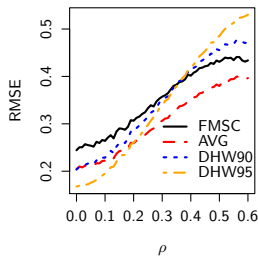
$N = 100, \pi = 0.2$



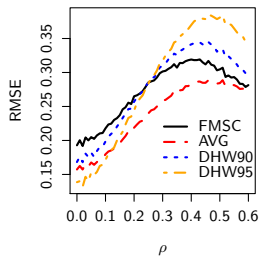
$N = 500, \pi = 0.2$



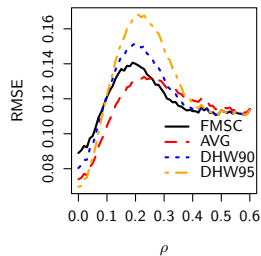
$N = 50, \pi = 0.4$



$N = 100, \pi = 0.4$



$N = 500, \pi = 0.4$



Choosing Instrumental Variables Simulation

$$y_i = 0.5x_i + \epsilon_i$$

$$x_i = (z_{1i} + z_{2i} + z_{3i})/3 + \gamma w_i + v_i$$

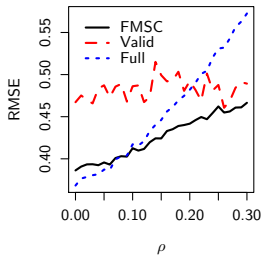
$$(\epsilon_i, v_i, w_i, z_{1i}, z_{2i}, z_{3i})' \sim \text{iid } N(0, \mathcal{V})$$

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

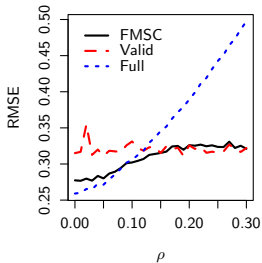
$$\gamma = \text{Cor}(x, w), \quad \rho = \text{Cor}(w, \epsilon), \quad \text{First-Stage } R^2 = 1/9 + \gamma^2$$

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

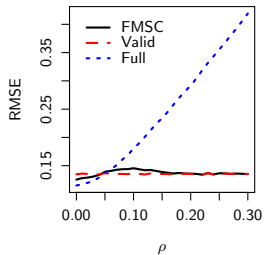
$N = 50, \gamma = 0.2$



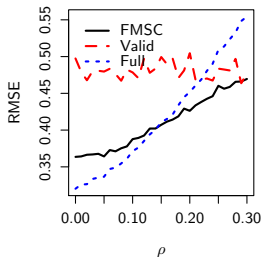
$N = 100, \gamma = 0.2$



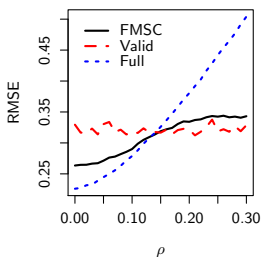
$N = 500, \gamma = 0.2$



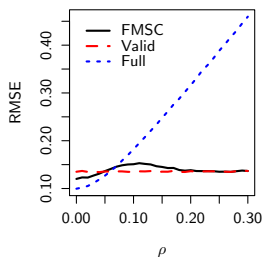
$N = 50, \gamma = 0.3$



$N = 100, \gamma = 0.3$



$N = 500, \gamma = 0.3$



Alternative Moment Selection Procedures

Downward J -test

Use Full instrument set unless J -test rejects.

Andrews (1999) – GMM Moment Selection Criteria

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

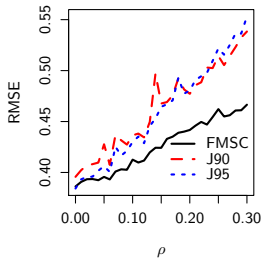
Hall & Peixe (2003) – Canonical Correlations Info. Criterion

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

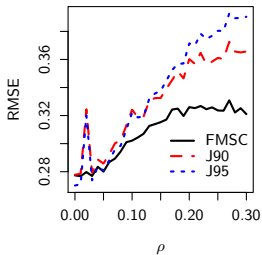
Penalty/Bonus Terms

Analogies to AIC, BIC, and Hannan-Quinn

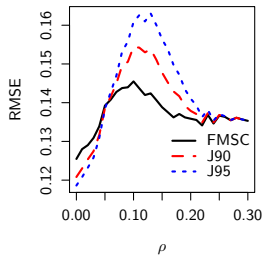
$N = 50, \gamma = 0.2$



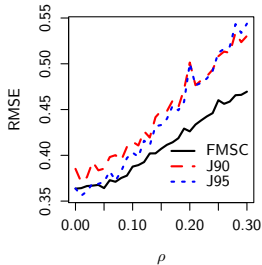
$N = 100, \gamma = 0.2$



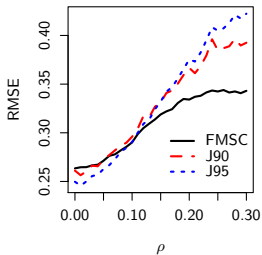
$N = 500, \gamma = 0.2$



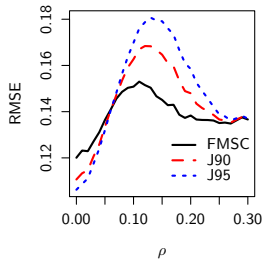
$N = 50, \gamma = 0.3$



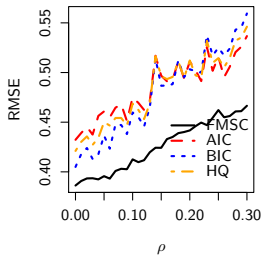
$N = 100, \gamma = 0.3$



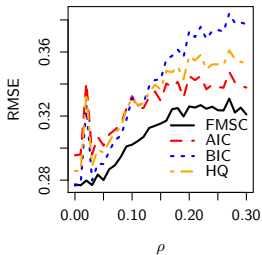
$N = 500, \gamma = 0.3$



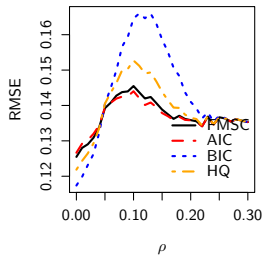
$N = 50, \gamma = 0.2$



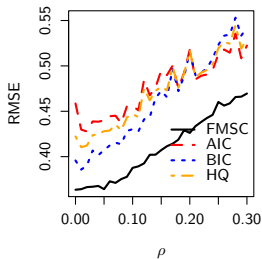
$N = 100, \gamma = 0.2$



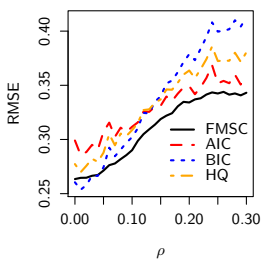
$N = 500, \gamma = 0.2$



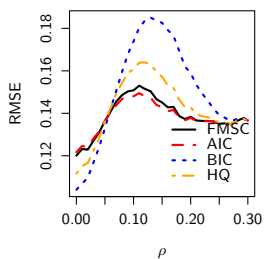
$N = 50, \gamma = 0.3$



$N = 100, \gamma = 0.3$



$N = 500, \gamma = 0.3$



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

- ▶ *Inmort* – 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*

	$\mu = \text{malfal}$			$\mu = \text{rule}$		
	FMSC	posFMSC	$\hat{\mu}$	FMSC	posFMSC	$\hat{\mu}$
(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 #8 – High-Dimensional Regression I

The James-Stein Estimator

QR Decomposition

Singular Value Decomposition

Review of Principal Component Analysis (PCA)

Recall: Gauss-Markov Theorem

Linear Regression Model

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

Best Linear Unbiased Estimator

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

What if we consider biased estimators?

Dominance and Admissibility

Notation

Let R be a risk function, e.g. MSE, and $\hat{\theta}$ and $\tilde{\theta}$ be estimators of θ .

Dominance

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

Admissibility

We say that $\hat{\theta}$ is **admissible** if no other estimator dominates it.

Inadmissibility

To prove that an estimator $\tilde{\theta}$ is **inadmissible** it suffices to find an estimator $\hat{\theta}$ that dominates it.

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

Goal

Estimate the p -vector of unknown parameters θ using X .

Maximum Likelihood Estimator $\hat{\theta}$

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

MSE of $\hat{\theta}$

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

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

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

James-Stein Estimator

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

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

MSE of James-Stein Estimator

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

Using fact that $MSE(\hat{\theta}) = p$

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 $i = 1, \dots, p$

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

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 $p \geq 3$

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

- ▶ $\mathbb{E}[1/(X'X)]$ 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:

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

- ▶ $\hat{\beta} = \text{OLS}$, $(x)_+ = \max(x, 0)$, $\hat{\sigma}^2 = \text{usual OLS-based estimator}$
- ▶ Stops 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!

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 $X = QR$

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

In other words, $\hat{\beta}$ 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 j th column of A .
 - ▶ Let \mathbf{e}_j be the j th standard basis vector.
 - ▶ Inverting R is equivalent to solving $R\mathbf{a}_1 = \mathbf{e}_1$, followed by $R\mathbf{a}_2 = \mathbf{e}_2, \dots, R\mathbf{a}_k = \mathbf{e}_k$.
- ▶ 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

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

- ▶ $U = m \times m$ orthog. matrix whose cols contain e-vectors of AA'
- ▶ $V = n \times n$ orthog. matrix whose cols contain e-vectors of $A'A$
- ▶ $D = m \times n$ matrix whose first r main diagonal elements are the *singular values* d_1, \dots, d_r . All other elements are zero.
- ▶ The singular values d_1, \dots, 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 $d_1 \leq d_2 \leq \dots \leq d_r$
- ▶ 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

$$\alpha_1 = \arg \max_{\alpha} \text{Var}(\alpha' \mathbf{x}) \quad \text{subject to} \quad \alpha' \alpha = 1$$

First Principal Component

The linear combination $\alpha_1' \mathbf{x}$ is the **first principal component** of \mathbf{x} .

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

Solving for α_1

Lagrangian

$$\mathcal{L}(\alpha_1, \lambda) = \alpha' \Sigma \alpha - \lambda(\alpha' \alpha - 1)$$

First Order Condition

$$2(\Sigma \alpha_1 - \lambda \alpha_1) = 0 \iff (\Sigma - \lambda I_p) \alpha_1 = 0 \iff \Sigma \alpha_1 = \lambda \alpha_1$$

Variance of 1st PC

α_1 is an e-vector of Σ but which one? Substituting,

$$\text{Var}(\alpha'_1 \mathbf{x}) = \alpha'_1 (\Sigma \alpha_1) = \lambda \alpha'_1 \alpha_1 = \lambda$$

Solution

Var. of 1st PC equals λ and this is what we want to **maximize**, so

α_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 $\alpha'_2 \mathbf{x}$ is uncorrelated with $\alpha'_1 \mathbf{x}$.

j th Principal Component

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

Sample PCA

Notation

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

SVD

$$X = UDV', \text{ thus } X'X = VDU'UDV' = VD^2V'$$

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 j th column of V . Then,

\mathbf{v}_j = PC loadings for j th PC of S

$\mathbf{v}_j' \mathbf{x}_i$ = PC score for individual/time period i

Sample PCA

PC scores for j th 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.

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

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 $X'X = VD^2V'$

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

Lecture #9 – High-Dimensional Regression II

Ridge Regression

LASSO

Ridge Regression – OLS with an L_2 Penalty

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

- ▶ Add a penalty for large coefficients
- ▶ λ = 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

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

- ▶ 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-dependend)

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,

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

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

Ridge Regression via OLS with “Dummy Observations”

Ridge regression solution is identical to

$$\arg \min_{\beta} \left(\tilde{\mathbf{y}} - \tilde{X}\beta \right)' \left(\tilde{\mathbf{y}} - \tilde{X}\beta \right)$$

where

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

since:

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

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:

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

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

Columns of $\sqrt{\lambda} I_p$ are linearly independent, so columns of \tilde{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 $\tilde{X} = QR$ so

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

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

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 $X_{(n \times p)}$ with rank p so OLS estimator is unique.

Economical SVD

- ▶ $X_{(n \times p)} = U_{(n \times p)} D_{(p \times p)} V'_{(p \times p)}$ 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 and U are square orthogonal,

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

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 $H(\lambda)$

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

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

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

Effective Degrees of Freedom for Ridge Regression

Using cyclic permutation property of trace:

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

- ▶ $\text{df}(\lambda) \rightarrow 0$ as $\lambda \rightarrow 0$
- ▶ $\text{df}(\lambda) = p$ when $\lambda = 0$
- ▶ $\text{df}(\lambda) < p$ when $\lambda > 0$

Comparing OLS and Ridge Predictions

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

Comparing OLS and Ridge Predictions

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

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

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

- ▶ 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: $\mathbf{z}_j = d_j \mathbf{u}_j$.
3. Throw away all but first M principal components, where $M < p$.
4. Regress \mathbf{y} on $\mathbf{z}_1, \dots, \mathbf{z}_k$.

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

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

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

LASSO – L_1 Penalty

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

Other Ways of Thinking about LASSO

Constrained Optimization

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

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

Bayesian Posterior Mode

Ignoring the intercept, LASSO is the posterior 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 $\text{Lap}(x|\mu, \tau) = (2\tau)^{-1} \exp \{-\tau^{-1}|x - \mu|\}$

Comparing Ridge and LASSO – Bayesian Posterior Modes

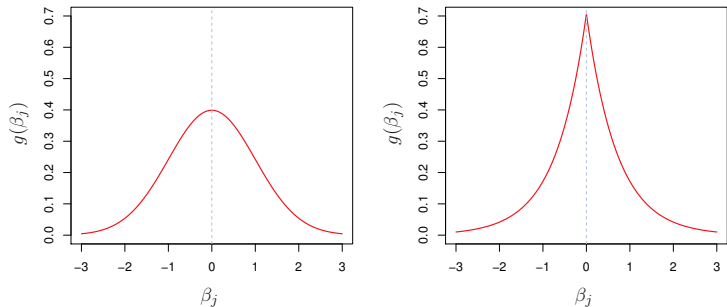


Figure: Ridge, at left, puts a normal prior on β while LASSO, at right, uses a Laplace prior, which has fatter tails and a taller peak at zero.

Comparing LASSO and Ridge – Constrained OLS

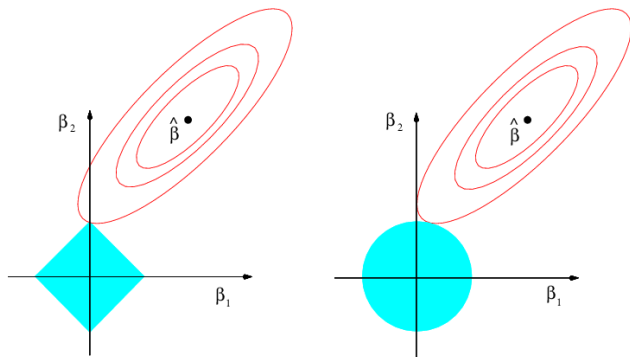


Figure: $\hat{\beta}$ denotes the MLE and the ellipses are the contours of the likelihood. LASSO, at left, and Ridge, at right, both shrink β away from the MLE towards zero. Because of its diamond-shaped constraint set, however, LASSO favors a **sparse solution** while Ridge does not

No Closed-Form for LASSO!

Simple Special Case

Suppose that $X'X = I_p$

Maximum Likelihood

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

Ridge Regression

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

So what about LASSO?

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

Want to Solve

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

Expand First Term

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

Hence

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

LASSO when $X'X = I_p$

Preceding Slide

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

Key Simplification

Equivalent to solving j independent optimization problems:

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

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

LASSO when $X'X = I_p$

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

Optimization problem becomes

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

Interior solution:

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

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

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

LASSO when $X'X = I_p$

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

Optimization problem becomes

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

Interior solution:

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

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

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

Ridge versus LASSO when $X'X = I_p$

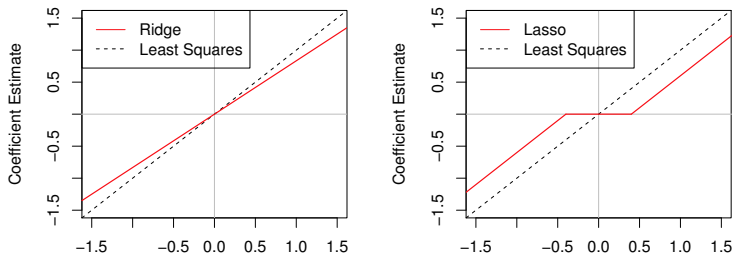


Figure: Horizontal axis in each plot is MLE

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

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

Calculating LASSO – The Shooting Algorithm

Cyclic Coordinate Descent

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

Result: LASSO Solution

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

repeat

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

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

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

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

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

end

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