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

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

Properties

- *Not* symmetric: $\mathrm{KL}(g;f) \neq \mathrm{KL}(f;g)$
- By Jensen's Inequality: $\mathrm{KL}(g;f) \geq 0$ (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

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

What if f_θ is correctly specified?

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

Goal: Compare Mis-specified Models

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

where θ_0 is the pseudo-true parameter value for f_θ and γ_0 is the pseudo-true parameter value for h_γ.

How to Estimate Expected Log Likelihood?

For simplicity: $Y_1, \ldots, Y_n \sim$ iid $g(y)$

Unbiased but Infeasible

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

Biased but Feasible

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

Intuition for the Bias

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

What to do about this bias?

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

Tradeoffs

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

Recall: Asymptotics for Mis-specified ML Estimation

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

Fundamental Expansion

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

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

Central Limit Theorem

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

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

Information Matrix Equality

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

Bias Relative to Infeasible Plug-in Estimator

Definition of Bias Term B

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

Question to Answer

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

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

Derivation of AIC/TIC

Step 1: Taylor Expansion

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

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

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

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

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

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

Derivation of AIC/TIC Continued...

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

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

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

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

Final Result:

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

TIC and AIC

Takeuchi's Information Criterion

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

Akaike's Information Criterion

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

Contrasting AIC and TIC

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

Corrected AIC (AIC$_c$) – Hurvich & Tsai (1989)

Idea Behind AIC$_c$

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

Assumption: True DGP

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

Can Show That

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

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

But how can we use this?

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

1. Would need to know (β_1, σ_1^2) for candidate model.
   - Easy: just use MLE $(\widehat{\boldsymbol{\beta}}_1, \widehat{\sigma}_1^2)$
2. Would need to know $(\boldsymbol{\beta}_0, \sigma_0^2)$ for true model.
   - Very hard! The whole problem is that we don't know these!

Hurvich & Tsai (1989) Assume:

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

Deriving the Corrected AIC

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

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

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

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

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

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

a finite-sample unbiased estimator of KL for model comparison

Lecture #2 – More on “Classical” Model Selection

Mallow’s C_p

Bayesian Model Comparison

Laplace Approximation

Bayesian Information Criterion (BIC)

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

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

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

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

Operationalizing the Bias-Variance Tradeoff Idea

Mallow's C_p

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

Notation

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

In-sample versus Out-of-sample Prediction Error

Why not compare RSS(m)?

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

From your Problem Set

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

Bias-Variance Tradeoff

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

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

Step 1: Algebra

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

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

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

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

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 $\widehat{\boldsymbol{\beta}}$ 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...

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

Therefore:

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

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

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

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

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...

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

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

Use to Approximate Marginal Likelihood

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

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

Laplace Approximation to Marginal Likelihood

Suppress model index m for simplicity.

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

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

Bayesian Information Criterion

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

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:

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

large-sample Frequentist approx. to Bayesian marginal likelihood

Lecture #3 – Cross-Validation

Model selection via a Hold-out Sample

K-fold Cross-validation

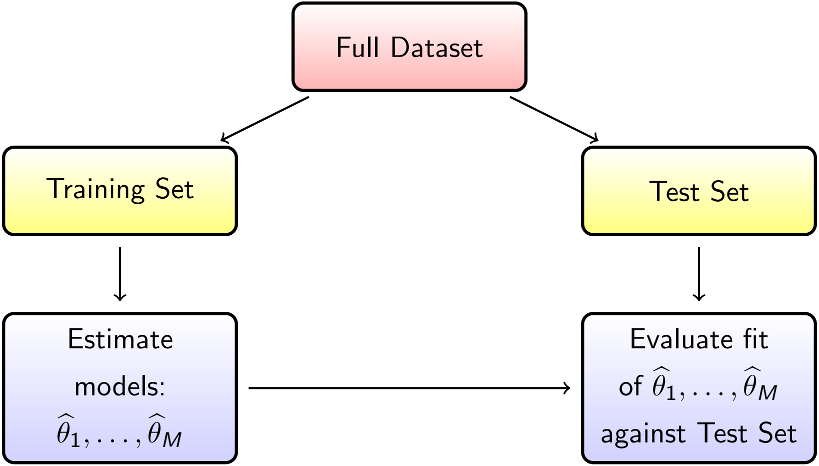
Asymptotic Equivalence Between LOO-CV and TIC

Influence Functions

Model Selection using a Hold-out Sample

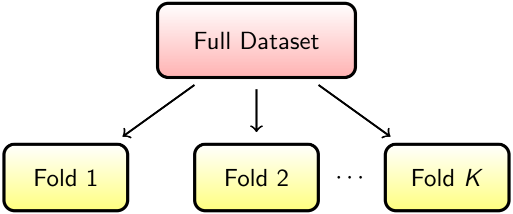
- The real problem is double use of the data: first for estimation, then for model comparison.
  - Maximized sample log-likelihood is an overly optimistic estimate of expected log-likelihood and hence KL-divergence
  - In-sample squared prediction error is an overly optimistic estimator of out-of-sample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

Hold-out Sample: Partition the Full Dataset



Unfortunately this is extremely wasteful of data. . .

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



Step 1

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

Step 2

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

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

Step 2

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

Step 3

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

Step 4

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

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

Step 4

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

Step 5

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

Step 5

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

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

Cross-Validation (CV): Some Details

Which Loss Function?

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

How Many Folds?

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

Relationship between LOO-CV and TIC

Theorem

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

Large-sample Equivalence of LOO-CV and TIC

Notation and Assumptions

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

Log-likelihood as "Loss"

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

Overview of the Proof

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

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

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

Overview of Proof

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

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

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

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

Overview of Proof

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

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

So it suffices to show that

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

Digression: Functionals and Influence Functions

(Statistical) Functional

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

Example: ML Estimation

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

Influence Function

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

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

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

Back to the Proof...

Step 1

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

Step 2

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

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

Step 3

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

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

Lecture #4 – Asymptotic Properties

Overview

Weak Consistency

Consistency

Efficiency

AIC versus BIC in a Simple Example

Overview

- What happens as $T \to \infty$?
- 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:

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

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

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

True DGP

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

Candidate Models

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

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

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

Log-Likelihood Function

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

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

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

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

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

Information Criteria

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

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

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

Difference of Criteria

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

Selected Model

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

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

$$
\begin{aligned}
\mathrm{KL}(g; \mathrm{M}_0) &= \int_{\mathbb{R}} \mu(y - \mu/2)(2\pi)^{-1/2} \exp\left\{(y-\mu)^2/2\right\}\, \mathrm{d}y \\
&= \mu(\mu - \mu/2) = \mu^2/2
\end{aligned}
$$

Verifying Weak Consistency: $\mu \neq 0$

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 $T \to \infty$.

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

Finite-Sample Selection Probabilities: AIC

AIC Sets $d_T = 2$

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

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

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

Finite-Sample Selection Probabilities: BIC

BIC sets $d_T = \log(T)$

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

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

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

Interactive Demo: AIC vs BIC

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

Probability of Over-fitting

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

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

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

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

Risk of the Post-Selection Estimator

The Post-Selection Estimator

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

Recall from above

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

Risk Function

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

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

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 $A = \left\{|\sqrt{T}\mu + Z| \geq \sqrt{d_T}\right\}$

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

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:

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

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

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

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

Therefore:

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

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

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

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

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

The Simplifed 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

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

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

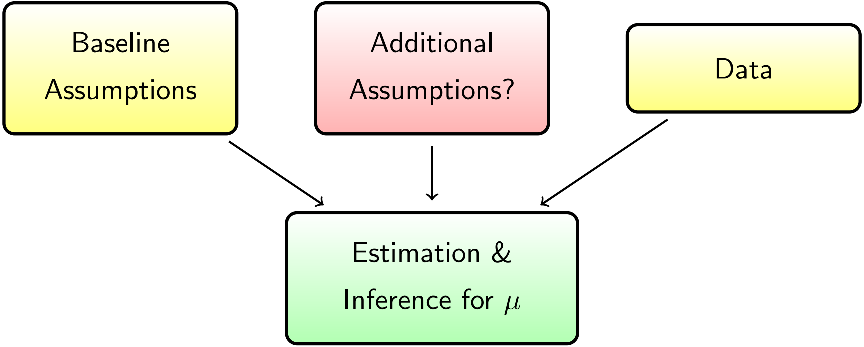
Punchline: Risk of the Post-Selection Estimator

- AIC: bounded worst-case risk
- BIC: low risk in a neighborhood of $\mu = 0$ in exhange 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

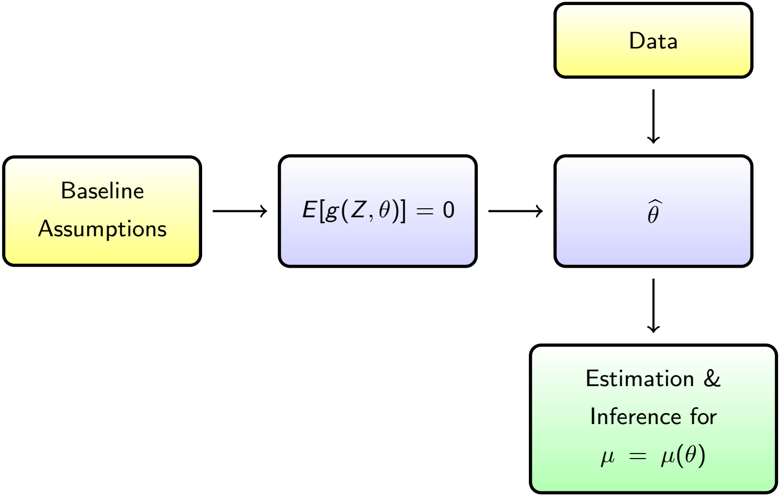
DiTraglia (2016, JoE)

Focused Moment Selection Criterion (FMSC)

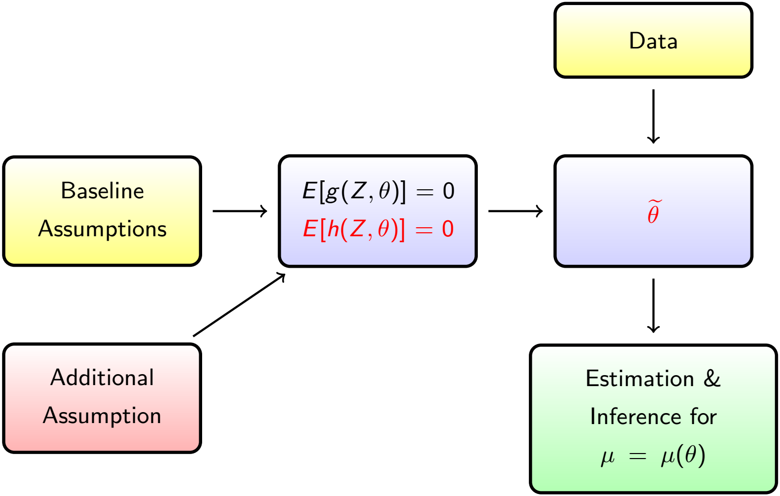


1. Choose False Assumptions on Purpose
2. Focused Choice of Assumptions
3. Local mis-specification
4. Averaging, Inference post-selection

GMM Framework



Adding Moment Conditions



Ordinary versus Two-Stage Least Squares

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

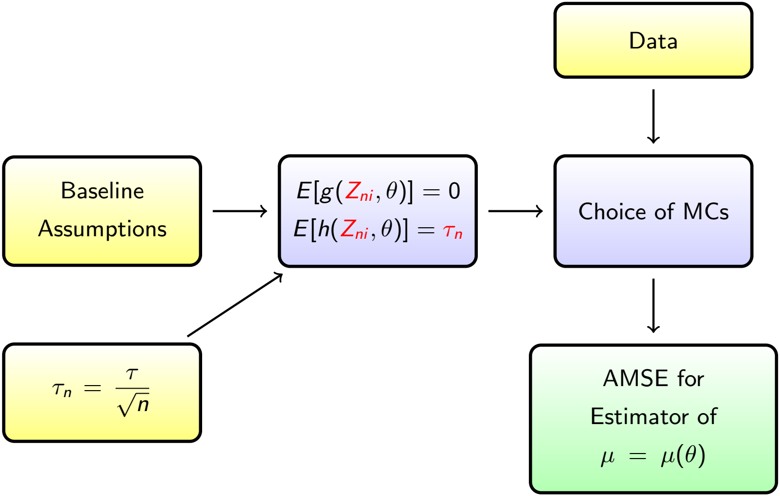
$$\begin{aligned} E[\mathbf{z}_i \epsilon_i] &= 0 \\ E[x_i \epsilon_i] &= ? \end{aligned}$$

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

Shorthand: Write Z for Z_i

Candidate GMM Estimator

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

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

Notation: Limit Quantities

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

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

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

Local Mis-Specification + Standard Regularity Conditions

Every candidate estimator is consistent for θ_0 and

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

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

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

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

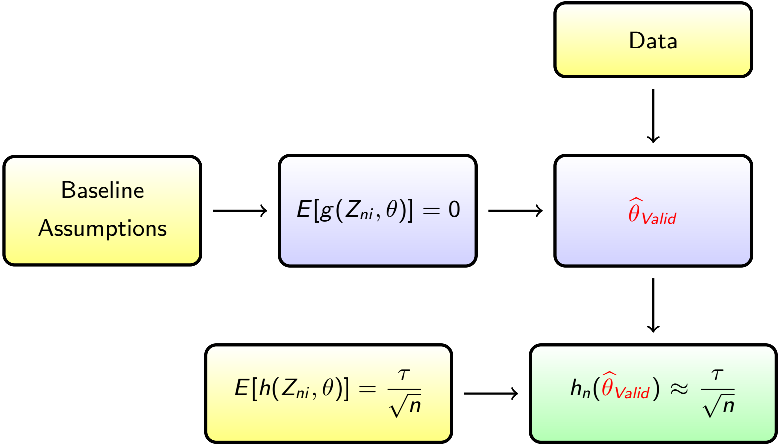
FMSC: Estimate AMSE($\widehat{\mu}_S$) and minimize over S

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

Estimating the unknowns

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

A Plug-in Estimator of τ



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

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

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

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

FMSC: Asymptotically Unbiased Estimator of AMSE

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

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

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

$FMSC_n(S) \to_d FMSC_S$, where

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

Conservative criterion: random even in the limit.

Moment Average Estimators

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

Additional Notation

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

Examples of Moment-Averaging Weights

Post-Moment Selection Weights

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

Exponential Weights

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

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

Two-step Procedure for Conservative Intervals

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

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

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

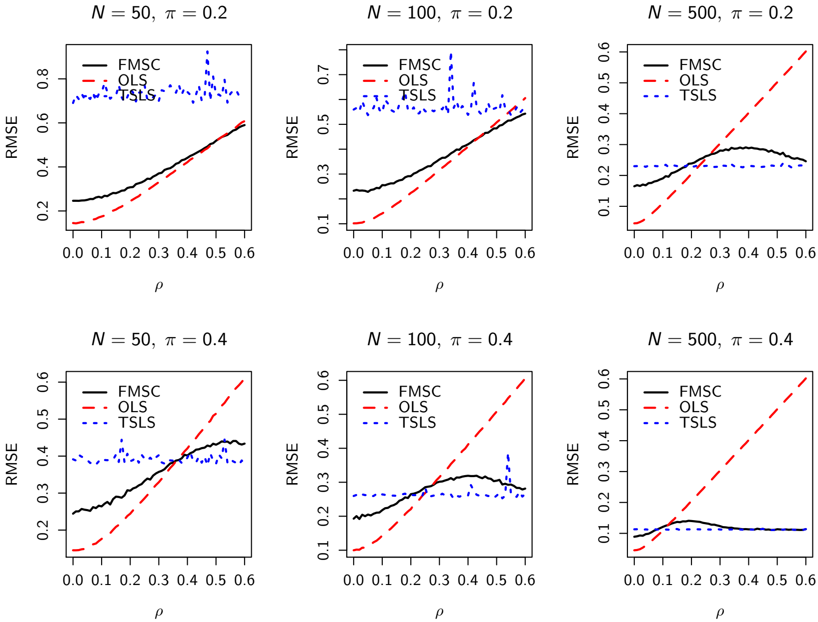
OLS versus TSLS Simulation

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

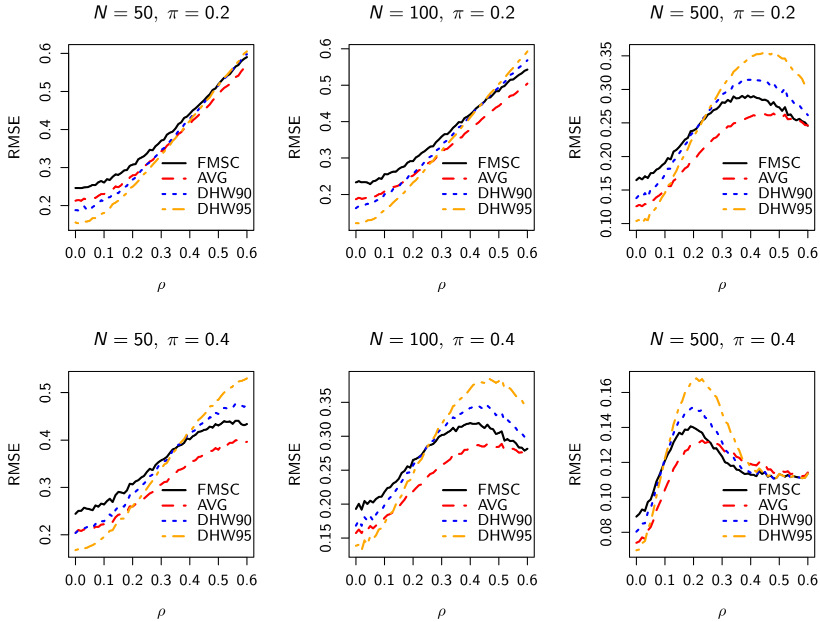
$$(\epsilon_i, v_i, z_{1i}, z_{2i}, z_{3i}) \sim \text{ iid } N(0, \mathcal{S})$$

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

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



$N = 50,\ \pi = 0.2$
$N = 100,\ \pi = 0.2$
$N = 500,\ \pi = 0.2$
$N = 50,\ \pi = 0.4$
$N = 100,\ \pi = 0.4$
$N = 500,\ \pi = 0.4$
FMSC
OLS
TSLS
RMSE
ρ



$N = 50,\ \pi = 0.2$
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$N = 500,\ \pi = 0.2$
$N = 50,\ \pi = 0.4$
$N = 100,\ \pi = 0.4$
$N = 500,\ \pi = 0.4$
RMSE
ρ
FMSC
AVG
DHW90
DHW95

Choosing Instrumental Variables Simulation

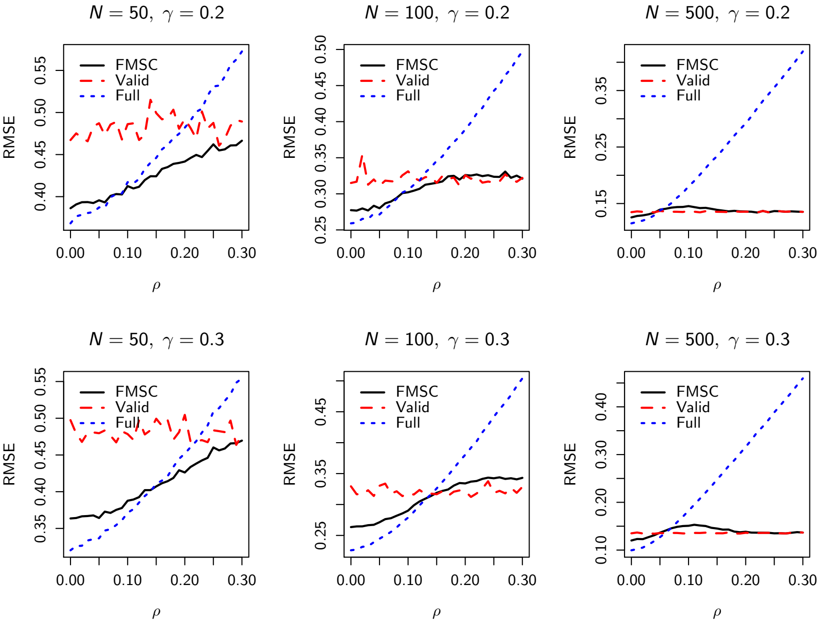
$$\begin{aligned} y_i &= 0.5x_i + \epsilon_i \\ x_i &= (z_{1i} + z_{2i} + z_{3i})/3 + \gamma w_i + v_i \end{aligned}$$

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

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

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

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



$N = 50,\ \gamma = 0.2$
$N = 100,\ \gamma = 0.2$
$N = 500,\ \gamma = 0.2$
$N = 50,\ \gamma = 0.3$
$N = 100,\ \gamma = 0.3$
$N = 500,\ \gamma = 0.3$
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

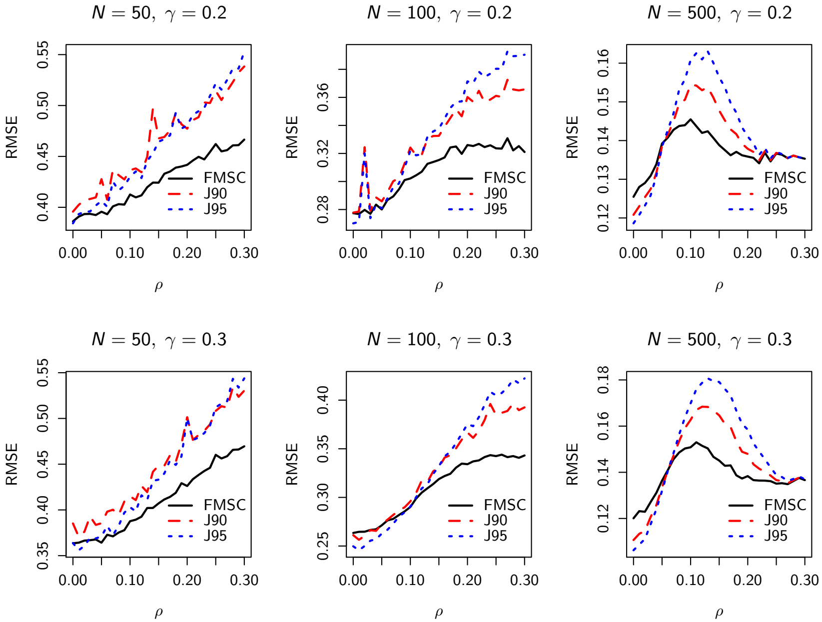
$\text{GMM-MSC}(S) = J_n(S) - \text{Bonus}$

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

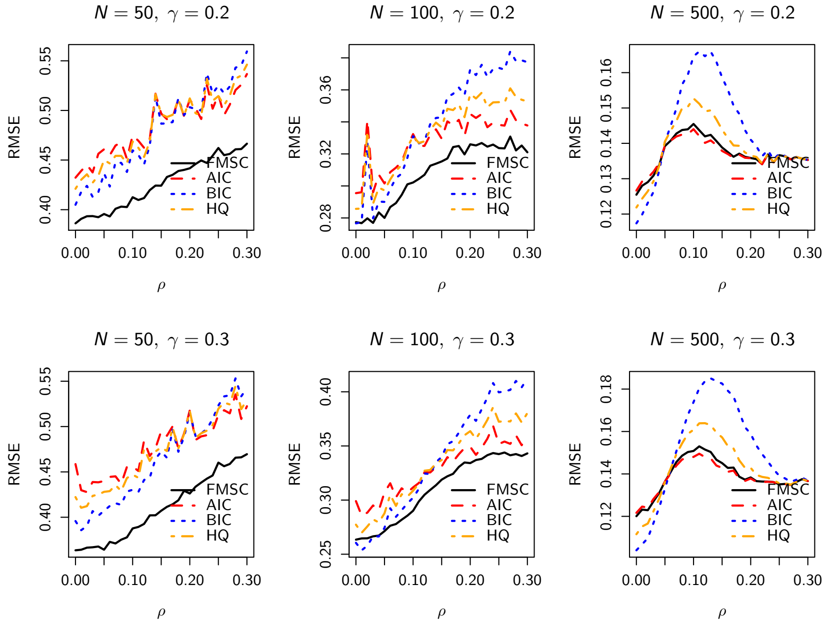
$\text{CCIC}(S) = n \log \left[1 - R_n^2(S)\right] + \textit{Penalty}$

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 #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

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

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?

Dominance and Admissibility

Notation

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

Dominance

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

Admissibility

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

Inadmissiblility

To prove that an estimator $\widetilde{\theta}$ is **inadmissible** it suffices to find an estimator $\widehat{\theta}$ 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 $\widehat{\theta}$

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

MSE 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 $MSE(\hat{\theta}) = p$.

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 ($\widehat{\theta}'\widehat{\theta}$ small) gives more shrinkage

MSE of James-Stein Estimator

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

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

Simplifying the Second Term

Writing Numerator as a Sum

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

For $i = 1, \ldots, p$

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

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

Combining

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

The MLE is Inadmissible when $p \geq 3$

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

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

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

James-Stein More Generally

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

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

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

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

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

- $U = m \times m$ 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

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

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 $X'X = VD^2V'$

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

Lecture #9 – High-Dimensional Regression II

Ridge Regression

Principal Components Regression

LASSO

Ridge Regression – OLS with an L_2 Penalty

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

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

Alternative Formulation of Ridge Regression Problem

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

- 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,

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

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 and U are square orthogonal,

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

Model Complexity of Ridge Versus OLS

OLS Case

Number of free parameters equals number of parameters p.

Ridge is more complicated

Even though there are p parameters they are constrained!

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

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

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

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

Effective Degrees of Freedom for Ridge Regression

Using cyclic permutation property of trace:

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

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

Comparing OLS and Ridge Predictions

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

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 M principal components, where $M < p$.
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

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

$\arg\min_{\beta} (\mathbf{y} - X\beta)'(\mathbf{y} - X\beta) \quad$ 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 $\text{Lap}(x|\mu, \tau) = (2\tau)^{-1} \exp\left\{-\tau^{-1}|x - \mu|\right\}$

Comparing Ridge and LASSO – Bayesian Posterior Modes

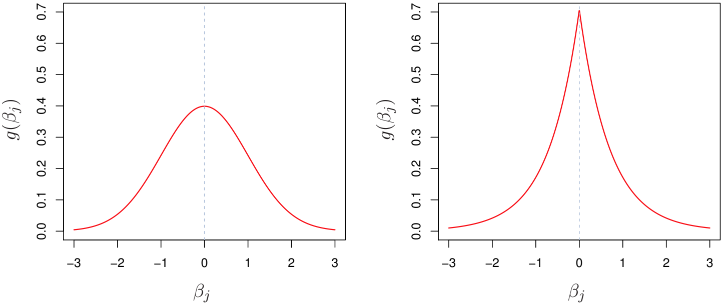


Figure: Ridge, at left, puts a normal prior on β while LASSO, at right, uses a Laplace prior, which has fatter tails and a taller peak at zero.

Comparing LASSO and Ridge – Constrained OLS

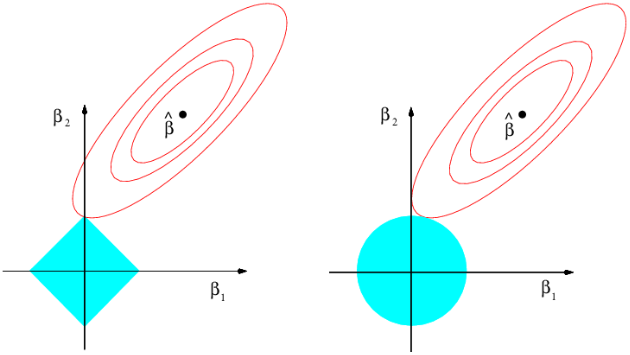


Figure: $\widehat{\beta}$ denotes the MLE and the ellipses are the contours of the likelihood. LASSO, at left, and Ridge, at right, both shrink β away from the MLE towards zero. Because of its diamond-shaped constraint set, however, LASSO favors a sparse solution while Ridge does not

No Closed-Form for LASSO!

Simple Special Case

Suppose that $X'X = I_p$

Maximum Likelihood

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

Ridge Regression

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

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

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

Key Simplification

Equivalent to solving j independent optimization problems:

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

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

LASSO when $X'X = I_p$

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

Optimization problem becomes

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

Interior solution:

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

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 $X'X = I_p$

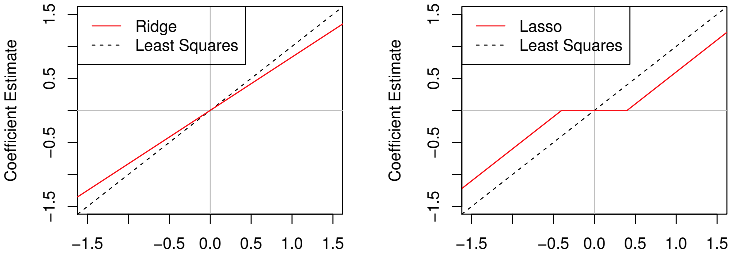


Figure: Horizontal axis in each plot is MLE

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

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

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

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

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

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

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

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

  end

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