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.

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

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Properties

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

KL Divergence and Mis-specified MLE

Pseudo-true Parameter Value θ_0

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

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What if f_θ is correctly specified?

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

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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

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

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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)
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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

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Fundamental Expansion

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

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

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Central Limit Theorem

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

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

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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

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

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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

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

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Derivation of AIC/TIC Continued...

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

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

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

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

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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.

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Assumption: True DGP

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

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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?

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   - Easy: just use MLE $(\widehat{\boldsymbol{\beta}}_1, \widehat{\sigma}_1^2)$
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   - Very hard! The whole problem is that we don't know these!

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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

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

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

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

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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

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

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

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- 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.

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

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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.

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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

$$\mathbf{X}\widehat{\boldsymbol{\beta}}_m - \mathbf{X}\boldsymbol{\beta} \quad = \quad \mathbf{P}_m\mathbf{y} - \mathbf{X}\boldsymbol{\beta}$$

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\end{aligned}$$

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

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

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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

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

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

Step 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 $\mathbf{X}\widehat{\beta}_m$ relative to infeasible optimum $\boldsymbol{X}\beta$

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

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

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 $\mathbf{X}$

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

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

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

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

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

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

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

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

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

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...

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

Bias-Variance Tradeoff

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.

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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.

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Mallow's C_p

- Problem: MSE formula is infeasible since it involves $\boldsymbol{\beta}$ and σ^2.

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

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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.

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

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

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- 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: $\mathbf{X}\widehat{\beta} = \mathbf{Py}$.

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 $\mathbf{P}_m\mathbf{P} = \mathbf{P}\mathbf{P}_m = \mathbf{P}_m$.

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

Crucial Fact

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

Step 4: Algebra using the preceding fact

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

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

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

$$\mathbb{E}[\epsilon'(\mathbf{P} - \mathbf{P}_m)\epsilon|\mathbf{X}] = \mathbb{E}[\text{tr}\left\{\epsilon'(\mathbf{P} - \mathbf{P}_m)\epsilon\right\}|\mathbf{X}]$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Bias of Plug-in Estimator

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

Putting Everything Together: Mallow's C_p

Want An Unbiased Estimator of This:

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

Previous Slide:

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

Putting Everything Together: Mallow's C_p

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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...

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

Why is this different from the textbook formula?

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

Therefore:

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

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 $m \in \mathcal{M}$

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

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

Bayesian Model Comparison: Marginal Likelihoods

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

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

$$P(m|\mathbf{y}) = \frac{P(m) f(\mathbf{y}|m)}{f(\mathbf{y})} =$$

Bayesian Model Comparison: Marginal Likelihoods

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

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

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

Bayesian Model Comparison: Marginal Likelihoods

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

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

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

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

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

Laplace (aka Saddlepoint) Approximation

Suppress model index m for simplicity.

General Case: for T large...

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

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

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Use to Approximate Marginal Likelihood

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

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

Laplace Approximation to Marginal Likelihood

Suppress model index m for simplicity.

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

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

Bayesian Information Criterion

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

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Take Logs and Multiply by 2

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

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The BIC

Assume uniform prior over models and ignore lower order terms:

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

large-sample Frequentist approx. to Bayesian marginal likelihood

Lecture #3 – Cross-Validation

Model selection via a Hold-out Sample

K-fold Cross-validation

Asymptotic Equivalence Between LOO-CV and TIC

Influence Functions

Model Selection using a Hold-out Sample

- The real problem is double use of the data: first for estimation, then for model comparison.

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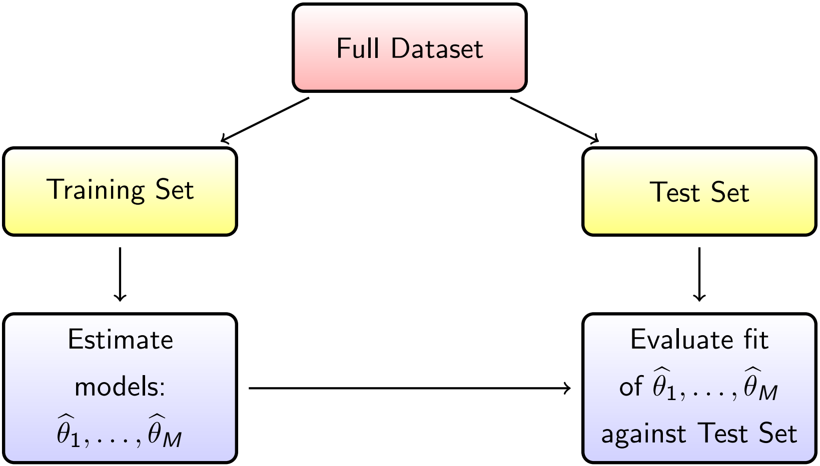
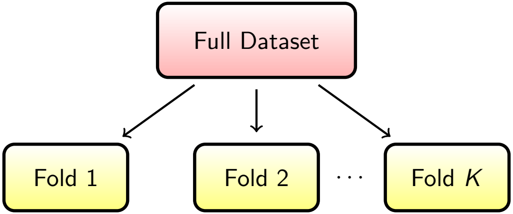
- AIC/TIC, AIC_c, BIC, C_p penalize sample log-likelihood or RSS to compensate.
- Another idea: don't re-use the same data!

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.

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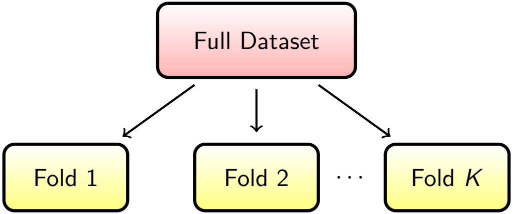

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Treat k^{th} fold as a hold-out sample and estimate model using all observations except those in fold k: yielding estimator $\widehat{\theta}(-k)$.

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

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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.

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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.

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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?

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- 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.

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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 $\widehat{\theta}$:

$$CV_1 = \frac{1}{T}\sum_{t=1}^{T} \log f(y_t|\widehat{\theta}_{(t)})$$

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\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)
\end{aligned}
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&= \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:

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

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&= \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]
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\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 $\mathbb{R}^p$.

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Example: ML Estimation

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

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

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Step 2

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

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

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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) \\
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Generic penalty $c_{T,k}$

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

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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

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

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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.

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Consequences

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- 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.

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

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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

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

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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*.

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- 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

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

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True DGP

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

$$\ell_T(\mu) \quad = \quad \sum_{t=1}^{T} \log\left(\frac{1}{2\pi}\exp\left\{-\frac{1}{2}(Y_t - \mu)^2\right\}\right)$$

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&= \text{Constant} - \frac{T}{2}(\bar{Y} - \mu)^2
\end{aligned}$$

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

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

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

Information Criteria

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

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

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

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.

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

Verifying Weak Consistency: $\mu \neq 0$

Condition on KL-Divergence

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

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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

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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 $d_T = 2$

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

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

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&= 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 $d_T = \log(T)$

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

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

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

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Interactive Demo: AIC vs BIC

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

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- AIC: $d_T = 2$ and $P(\chi^2_1 \geq 2) \approx 0.157$.

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- 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 $T \to 0$.

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

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

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Recall from above

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

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

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&= \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
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&= \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 $b = (\sqrt{d_T} - \sqrt{T}\mu)$

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&= \mathbb{P}(Z \geq b) + \mathbb{P}(Z \leq a) \\
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\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 $Z|X=1$

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

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

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Therefore:

$$\mathbb{P}(A)\,\mathbb{E}[Z^2|X=1] \;=\; \mathbb{P}(A)\int_{\mathbb{R}} z^2 \left[\frac{\mathbf{1}(A)\varphi(z)}{\mathbb{P}(A)}\right] \mathrm{d}z$$

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

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

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:

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

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

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

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

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

$$\int_a^b z^2\phi(z)\;dz \quad = \quad (2\pi)^{-1/2}\int_a^b z^2\exp\left\{-z^2/2\;\right\}\;\mathrm{d}z$$

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

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

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

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)