# MLR Model Selection

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*This material is part of the* **statsTeachR** *project*

# Today's Lecture

- Model selection vs. model checking
- Stepwise model selection
- Criterion-based approaches
- Cross-validation

# Model selection vs. model checking

Assume $y|\mathbf{x} = f(\mathbf{x}) + \epsilon$

- model selection focuses on how you construct $f(\cdot)$;
- model checking asks whether the $\epsilon$ match the assumed form.

# Why are you building a model in the first place?

# Model selection: considerations

## Things to keep in mind...

- **Why am I building a model?** Some common answers
  - Estimate an association
  - Test a particular hypothesis
  - Predict new values
- What predictors will I allow?
- What predictors are needed?
- What forms for $f(x)$ should I consider?

Different answers to these questions will yield different final models.

# Model selection: realities

*All models are wrong. Some are more useful than others.*
- George Box

- If we are asking which is the "true" model, we will have a bad time
- In practice, issues with sample size, collinearity, and available predictors are real problems
- It is often possible to differentiate between better models and less-good models, though

# Basic idea for model selection

## A very general algorithm

- Specify a "class" of models
- Define a criterion to quantify the fit of each model in the class
- Select the model that optimizes the criterion you're using
- Subject the selected model to model checking/diagnostics, possibly adjust interpretations as needed.

Again, we're focusing on $f(x)$ in the model specification. Once you've selected a model, you should subject it to regression diagnostics – which might change or augment the class of models you specify or alter your criterion.

# Classes of models

## Some examples of classes of models

- Linear models including all subsets of $x_1, ..., x_p$
- Linear models including all subsets of $x_1, ..., x_p$ and their first order interactions
- All functions $f(x_1)$ such that $f''(x_1)$ is continuous
- Additive models of the form $f(\mathbf{x}) = f_1(x_1) + f_2(x_2) + f_3(x_3)...$ where $f_k''(x_k)$ is continuous

# Popular criteria

- Adjusted $R^2$
- Residual mean square error
- Akaike Information Criterion (AIC)
- Bayes Information Criterion (BIC)
- Prediction RSS (PRESS)
- $F$- or $t$-tests (via stepwise selection)
- Likelihood ratio tests (F-tests)

# Adjusted $R^2$

- Recall:

$$R^2 = 1 - \frac{RSS}{TSS}$$

- Definition of adjusted $R^2$:

$$\begin{aligned} R_a^2 &= 1 - \frac{RSS/(n-p-1)}{TSS/(n-1)} = 1 - \frac{\hat{\sigma}^2_{model}}{\hat{\sigma}^2_{null}} \\ &= 1 - \frac{n-1}{n-p-1}(1-R^2) \end{aligned}$$

- Minimizing the standard error of prediction means minimizing $\hat{\sigma}^2_{model}$ which in turn means maximizing $R_a^2$
- Unlike with $R^2$, adding a predictor will not necessarily increase $R_a^2$ unless it has some predictive value

# Residual Mean Square Error

## Equivalent to Adjusted $R^2$...

$$RMSE = \frac{RSS}{n - p - 1}$$

Can choose either based on

- the model with minimum RMSE, or
- the model that has RMSE approximately equal to the MSE from the full model

Note: minimizing RMSE is equivalent to maximizing Adjusted $R^2$

# Sidebar: Confusing notation about $p$

## $p$ can mean different things

- $p$ can be the number of covariates you have in your model (not including your column of 1s and the intercept
- $p$ can be the number of betas you estimate, including $\beta_0$.

In these slides, $p$ is the former: the number of covariates.

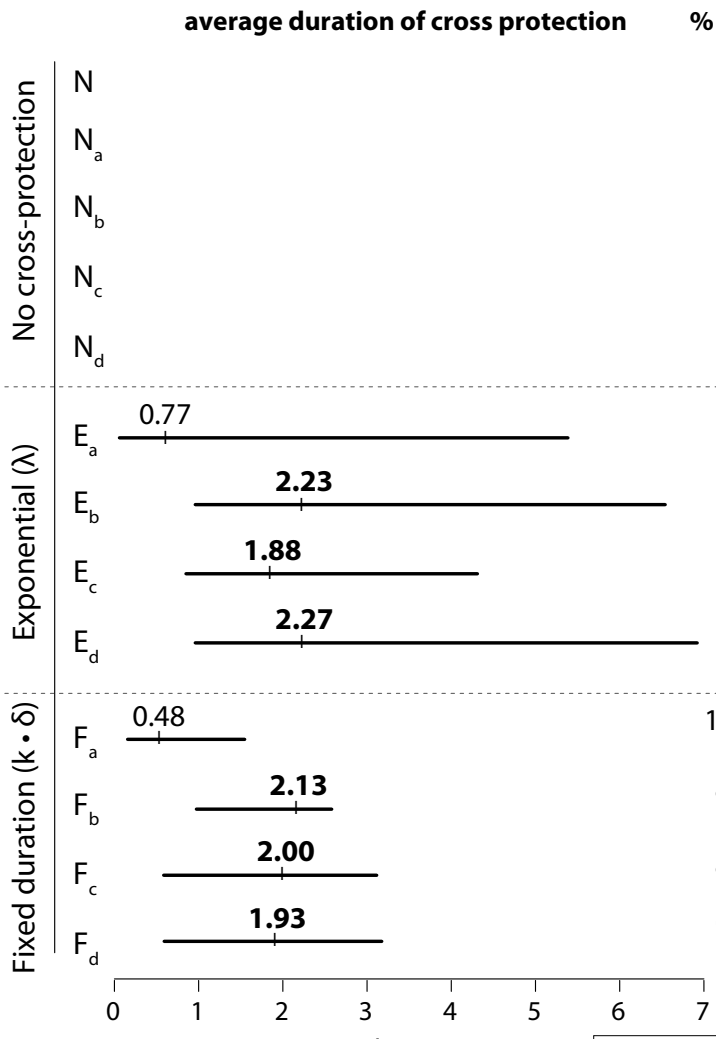
# AIC

AIC ("Akaike Information Criterion") measures goodness-of-fit through RSS (equivalently, log likelihood) and penalizes model size:

$$AIC = n \log(RSS/n) + 2(p+1)$$

- Small AIC's are better, but scores are not directly interpretable
- Penalty on model size tries to induce *parsimony*

# Example of AIC in practice




| | % protected (δ) | $r_i$* | r(t)* | loglik | df | ΔAIC |
|---|---|---|---|---|---|---|
| $N$ | 0 | | | -902.4 | 3 | 0 |
| $N_a$ | 0 | | | -946.7 | 15 | 112.6 |
| $N_b$ | 0 | • | | **-882.9** | **19** | **-7.0** |
| $N_c$ | 0 | | • | **-817.2** | **41** | **-94.4** |
| $N_d$ | 0 | • | • | **-781.1** | **119** | **-10.7** |
| $E_a$ | 100 | | | -943.3 | 16 | 107.7 |
| $E_b$ | **100** | • | | **-873.9** | **20** | **-23.1** |
| $E_c$ | **100** | | • | **-810.0** | **42** | **-106.9** |
| $E_d$ | **100** | • | • | **-773.5** | **120** | **-23.9** |
| $F_a$ | 100 (30 - 100) | | | -941.8 | 17 | 106.7 |
| $F_b$ | **84 (39 - 100)** | • | | **-870.5** | **21** | **-28.0** |
| $F_c$ | **80 (33 - 100)** | | • | **-807.3** | **43** | **-110.2** |
| $F_d$ | **76 (32 - 100)** | • | • | **-771.0** | **121** | **-26.8** |

$r_i$ = serotype-specific transmission parameters included
r(t) = seasonal transmission parameters included
loglik = log likelihood for the given model
df = degrees of freedom of the model
ΔAIC = change in Akaike Information Criterion over null model

Reich et al. (2013) *Journal of the Royal Society Interface*

# BIC

BIC ("Bayes Information Criterion") similarly measures goodness-of-fit through RSS (equivalently, log likelihood) and penalizes model size:

$$BIC = n \log(RSS/n) + (p+1) \log(n)$$

- Small BIC's are better, but scores are not directly interpretable
- AIC and BIC measure goodness-of-fit through RSS, but use different penalties for model size. They won't always give the same answer

Bonus link! Bolker on AIC vs. BIC

# Example of BIC in practice

| Step | Number of Predictors in Model | Breslow's Thickness | DCCD | Ulceration | Age | Nodal Status[a] | Localization | Gender | BIC |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 7 | <0.0001 | 0.0068 | 0.0009 | 0.0051 | 0.0371 | 0.1380 | 0.8052 | 1,657.8 |
| 2 | 6 | <0.0001 | 0.0069 | 0.0008 | 0.0050 | 0.0340 | 0.1035 | — | 1,650.9 |
| 3 | 5 | <0.0001 | 0.0011 | 0.0008 | 0.0054 | 0.0475 | — | — | 1,646.6 |
| 4 | 4 | <0.0001 | <0.0001 | 0.0005 | 0.0127 | — | — | — | 1,643.6 |
| 5 | 3 | <0.0001 | <0.0001 | 0.0002 | — | — | — | — | 1,642.9 |
| 6 | 2 | <0.0001 | <0.0001 | — | — | — | — | — | 1,649.8 |
| 7 | 1 | <0.0001 | — | — | — | — | — | — | 1,679.1 |

*p*-Values are for testing whether a hazard ratio equals 1; low BIC identifies best model.
[a]As determined by routine histopathology.
doi:10.1371/journal.pmed.1001604.t004

Vasantha and Venkatesan (2014) *PLoS ONE*

# Example of model selection in practice

**TABLE 2. Results of unrestricted longitudinal latent class analysis in the Medical Research Council 1946 National Survey of Health and Development (pooled sexes, $n = 3,272$)**

| | Three classes (LLCA*-3) | Four classes (LLCA-4) | Five classes (LLCA-5) |
|---|---|---|---|
| Sequential model comparisons ($T + 1$ classes vs. $T$ classes) | 3 vs. 2 | 4 vs. 3 | 5 vs. 4 |
| Log-likelihood value for model with $T + 1$ classes | –3,243.605 | –3,211.173 | –3,201.380 |
| Log-likelihood value for model with $T$ classes | –3,344.440 | –3,243.605 | –3,211.173 |
| –2 difference in log-likelihood | 201.669 | 64.863 | 19.587 |
| Difference in no. of parameters ($T + 1$ classes vs. $T$ classes) | 7 | 8 | 8 |
| Lo-Mendell-Rubin adjusted LRT* value | 198.171 | 63.877 | 19.289 |
| Lo-Mendell-Rubin adjusted LRT $p$ value | <0.0001 | <0.0001 | 0.0322 |
| Bootstrap LRT $p$ value | <0.01 | <0.01 | >0.50 |
| Chi-square goodness-of-fit tests | | | |
| Degrees of freedom | 43 | 36 | 29 |
| LRT $\chi^2$ | 123.588 | 58.725 | 39.138 |
| $p$ value | <0.0001 | 0.0098 | 0.0990 |
| Bootstrap $p$ value† | <0.01 | 0.02 | 0.11 |
| Pearson $\chi^2$ | 132.431 | 49.416 | 35.966 |
| $p$ value | <0.0001 | 0.0674 | 0.1746 |
| Bootstrap $p$ value† | <0.01 | 0.10 | 0.40 |
| Information criterion‡ | | | |
| Akaike's Information Criterion | 6,527.210 | 6,476.347 | *6,470.760* |
| Bayesian Information Criterion | 6,649.073 | *6,640.862* | 6,677.927 |
| Sample-size-adjusted Bayesian Information Criterion | 6,585.524 | *6,555.071* | 6,569.894 |
| Entropy | 0.856 | 0.913 | 0.897 |
| Condition number§ | $0.120E^{-03}$ | $0.783E^{-03}$ | $0.379E^{-03}$ |

* LLCA, longitudinal latent class analysis; LRT, likelihood ratio test.
† Bootstrap $p$ values were based on 200 resamples.
‡ Minimum values are shown in italic type.
§ Condition number = ratio of the largest eigenvalue to the smallest eigenvalue for the Fisher information matrix. Small values less than $10E^{-09}$ indicate problems with model identification.

Croudace et al (2003) *Amer J Epidemiology*

# Cross-validation estimates "out-of-sample" prediction error

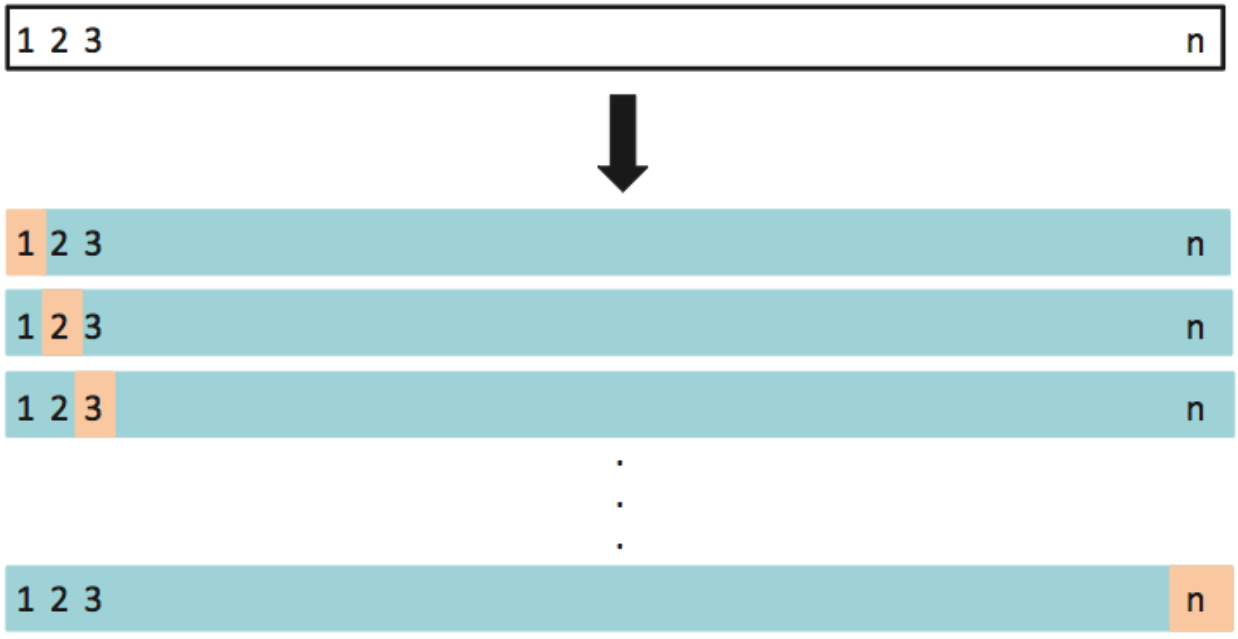



**FIGURE 5.3.** *A schematic display of LOOCV. A set of n data points is repeatedly split into a training set (shown in blue) containing all but one observation, and a validation set that contains only that observation (shown in beige). The test error is then estimated by averaging the n resulting MSE's. The first training set contains all but observation 1, the second training set contains all but observation 2, and so forth.*

More on cross-validation in *ISL* Chapter 5.

# Leave-one-out cross-validation, made simple

By fitting $n$ models, leaving one observation out sequentially, we could calculate the out-of-sample prediction error as:

$$CV_{(n)} = \frac{1}{n}\sum(y_i - \hat{y}_i^{(-i)})^2$$

This looks computationally intensive, but for linear regression models this is equivalent to

$$CV_{(n)} = \frac{1}{n}\sum\left(\frac{y_i - \hat{y}_i}{1 - h_{ii}}\right)^2$$

where the $\hat{y}$ come from the linear model fitted to all the data.
**No resampling needed!**

# k-fold cross-validation

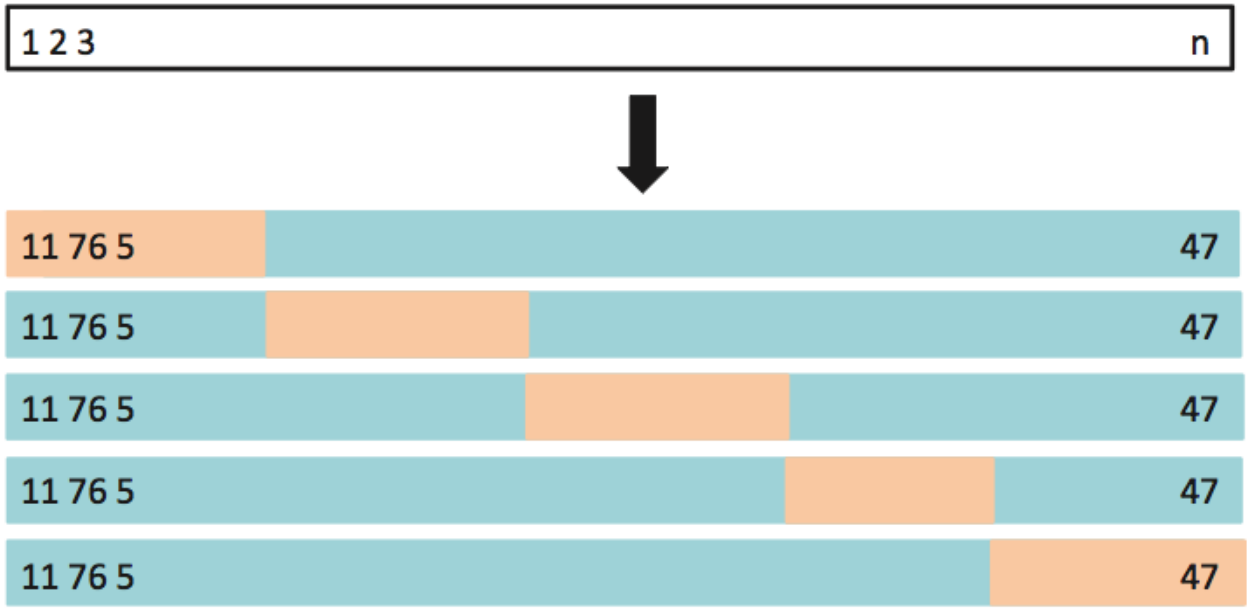



**FIGURE 5.5.** *A schematic display of 5-fold CV. A set of n observations is randomly split into five non-overlapping groups. Each of these fifths acts as a validation set (shown in beige), and the remainder as a training set (shown in blue). The test error is estimated by averaging the five resulting MSE estimates.*

Figure credits: *ISL* Chapter 5.

# k-fold cross-validation

As an alternative, we can fit $k$ models, by creating a random $k$-fold partition of your data,and calculate out-of-sample prediction error:

$$CV_{(k)} = \frac{1}{k} \sum_{i=1}^{k} MSE_i$$

where $MSE_i$ is the mean squared error of the observations in the $i^{th}$ held out fold.

Can be more computationally feasible when $n$ is large and you don't have the linear regression $h_i i$ computational shortcut.

# Why LOOCV can still lead to overfitting

Note: sums of highly correlated variables have high variance.

Which has a higher variance, $CV_{(k)}$ or $CV_{(n)}$?

Common choices for $k$ are 5 or 10.

# Model building is an art

Putting this all together requires

- knowledge of the process generating the data
- detailed data exploration
- checking assumptions
- careful model building
- patience patience patience

# Sequential variable selection methods

## PROCEED WITH CAUTION: Stepwise selection methods are dangerous if you want accurate inferences

- General idea: add/remove variables sequentially.
- There are many potential models – usually exhausting the model space is difficult or infeasible
- Stepwise methods don't consider all possibilities
- One paper* showed that stepwise analyses produced models that...
  - represented noise 20-75% of the time
  - contained <50% of actual predictors
  - correlation btw predictors $\longrightarrow$ including more predictors
  - number of predictors correlated with number of noise predictors included

* Derksen and Keselman (1992) *British J Math Stat Psych*

# MORE concerns with sequential methods

- It's common to treat the final model as if it were the only model ever considered – to base all interpretation on this model and to assume the inference is accurate
- This doesn't really reflect the true model building procedure, and can misrepresent what actually happened
- Inference is difficult in this case; it's hard to write down a statistical framework for the entire procedure
- Predictions can be made from the final model, but uncertainty around predictions will be understated
- P-values, CIs, etc will be incorrect

# Variable selection in polynomial models

A quick note about polynomials. If you fit a model of the form

$$y_i = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon_i$$

and find the quadratic term is significant but the linear term is not...

- You should still keep the linear term in the model
- Otherwise, your model is sensitive to centering – shifting $x$ will change your model
- Using orthogonal polynomials helps with this

# Variable selection: the intercept

A quick note about the intercept in MLR. If you fit a model of the form

$$y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + ... + \epsilon_i$$

and find the intercept term is not significant ...

- in general, you should still keep the intercept in the model
- Otherwise, your model is very strongly restricted in the linear form it can take!

# Sample size can limit the number of predictors

$p$ (total number of $\beta$s) should be $< \frac{m}{15}$, where

| Type of Response Variable | Limiting sample size $m$ |
|---|---|
| Continuous | $n$ (total sample size) |
| Binary | $min(n_1, n_2)$ |
| Ordinal ($k$ categories) | $n - \frac{1}{n^2} \sum_{i=1}^{k} n_i^3$ |
| Failure (survival) time | number of failures |

Table adapted from Harrel (2012) notes from "Regression Modeling Strategies" workshop.

# A more modern approach: shrinkage/penalization

## Penalized regression

- adds an explicit penalty to the least squares criterion
- keeps regression coefficients from being too large, or can shrink coefficients to zero
- Keywords for methods: LASSO, Ridge Regression
- More in Biostat Methods 3 (fall semester)!

Whole branches of modern statistics are devoted to figuring out what to do when $p \geq n$.

# Today's big ideas

## Model selection key points:

- There is no one-size-fits-all formula for model selection.
- Consult a variety of metrics, weight more heavily ones that may be more suited to your application (e.g. cross-validated metrics for prediction,...)
- Beware of black-box selection methods.
- Consider penalized regression methods.