Predictive Model Selection & Validation

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Model complexity

- In regression analyses, we can base model selection on a pre-specified set of predictor variables
  - variable selection which includes/excludes a particular variable ('best' subsets regression)
  - shrinkage methods which include all predictors but controls the size of the coefficients (one form of this is called ridge regression...more later!)
- Each approach employs a measure of 'complexity'
  - number of covariates
  - amount of control on the size of a coefficient
- Generically we will refer to this measure as a *tuning parameter*

Model complexity

- Determining a specific value for the tuning parameter is part of the model selection process
- For best subsets regression the tuning parameter is fairly easy to conceptualize, mainly because we can think in terms of the interpretation of predictors and their associated coefficients
- Other classes of restricted estimators also have associated measures of complexity
  - polynomial transformations
  - piecewise polynomials
  - natural cubic splines
  - smoothing splines

Model complexity

- Again, in each case we can still embed the choice of tuning parameter into the model selection process
  - in particular, we can view the determination of the level of complexity of our model as a model selection problem
- The selection process requires a means of assessing any given model
  - test or generalization error
  - error observed in an independent sample
- Our goal is to develop tools for the joint tasks of model assessment and selection

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Generalization performance

- We can formalize model assessment via a loss function and use expected prediction error, EPE, as a criterion for choosing a model
  - choose $f(\cdot)$ which minimizes EPE

$$f^*(\cdot) = \text{argmin}_{f(\cdot)} \, \mathrm{E}[L(Y, f(X))]$$

- Two examples of commonly considered loss functions are

1. Squared error (L_2) loss: $\mathrm{E}(Y - f(X))^2$
2. Absolute (L_1) loss: $\mathrm{E}|Y - f(X)|$

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Generalization performance

- L_2 loss is commonly used for many reasons, and in this case the we have $f^*(\cdot) = E[Y|\ X = x]$, the conditional expectation or regression function
- In this case there are many ways we can estimate $E[Y|\ X = x]$, and we would like a framework that can be used to assess, and order, competing choices.

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Generalization performance

- For a specified outcome variable Y and vector of predictor variables X, suppose we have a prediction model $\hat{f}(X)$, the form of which has been determined on the basis of a *training sample*
- We measure errors between Y and $\hat{f}(X)$ by specifying a loss function $L(Y, \hat{f}(X))$
- The *test* or *generalization* error is the expected prediction error over an *independent* test sample

$$\text{EPE} = \text{E}_{X,Y}\left[L(Y, \hat{f}(X))\right]$$

  - the expectation is taken over the joint distribution of X and Y
  - the average error, were the prediction model to be applied to an independent sample from the population

Generalization performance

- If we knew the true joint distribution of (X, Y), we could evaluate this expression directly
  - feasible in a simulation study where we know the truth
- However, in real life situations we won't know this joint distribution and so, for a given $\hat{f}(X)$, we need to estimate EPE
- A tempting choice could be the *training error*

$$\text{err} = \frac{1}{n}\sum_{i=1}^{n} L(y_i, \hat{f}(x_i))$$

Generalization performance

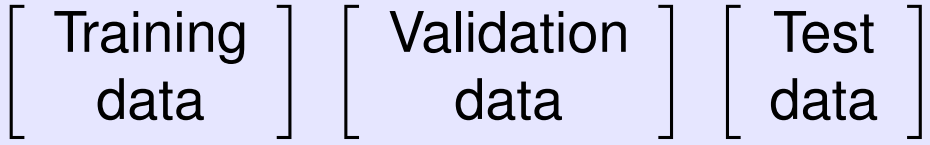
- Unfortunately the training error is not a good estimate of test error
  - the problem is that the estimate $\hat{y}_i = \hat{f}(x_i)$ uses y_i
  - the solution is specifically chosen because is does well in predicting the training data
- More specifically, the training error consistently decreases with model complexity
  - an extreme case is including a parameter for every observation (a *saturated* model), so that $\hat{f}(x_i) = y_i$ and there is zero training error!
- A model with zero training error can be viewed as an overfit to the training data and will typically generalize poorly
  - high sampling variability

Model assessment and selection

- We've already identified two separate goals we might have in mind: model selection and model assessment
- Model selection deals with estimating the performance of competing models in order to choose the best one
  - estimate the test error distribution across these models
  - choose the model which corresponds to the minimum
- Model assessment deals with evaluating the generalization error when applying the final model to new data
  - the final model is still chosen on the basis of the training data
  - seek an honest assessment of generalization error

Model assessment and selection

- In a data-rich situation, we could approach these goals jointly by splitting the data into three parts:



- Training data: *fit the models*
  - obtain point estimates for any given model under consideration
  - repeated use across models
- Validation data: *choose between models*
  - estimate the prediction error for model selection
  - repeated use across models
- Test data: *estimate generalization error of the final model*
  - one-time use, at the end of the analysis

Model assessment and selection

- Typically, we are not in a position to split the data into three parts
- A compromise might be to split the data into two parts

$$\left[\begin{array}{c}\text{Training}\\ \text{data}\end{array}\right] \quad \left[\begin{array}{c}\text{Test}\\ \text{data}\end{array}\right]$$

  and approximate the validation step
  - analytically: C_p, AIC and BIC
  - efficiency sample re-use: cross-validation and the bootstrap
- Even still, it may not be that splitting into two parts is feasible
  - consider whether or not these methods can be used to obtain reasonable assessments of generalization error

The bias-variance decomposition

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Squared error loss

- For a continuous outcome, suppose the data arise from the model

$$Y = f(X) + \epsilon$$

  - where $\mathrm{E}[\epsilon] = 0$ and $\mathrm{Var}[\epsilon] = \sigma^2$

- Under L_2 loss, the expected prediction error for an estimate $\hat{f}(\cdot)$ at $X = x_0$ can be decomposed as

$$\mathrm{EPE}(x_0) = \sigma^2 + \left\{\mathrm{E}[\hat{f}(x_0)] - f(x_0)\right\}^2 + \mathrm{Var}[\hat{f}(x_0)]$$

  - irreducible error + bias^2 + variance

The bias-variance decomposition

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Squared error loss

- This decomposition is specific to the L_2 loss but can be evaluated for any given estimator
- For linear regression we have

$$\text{EPE}(x_0) = \sigma^2 + \left\{ f(x_0) - \text{E}[\hat{f}(x_0)] \right\}^2 + ||\mathbf{h}(x_0)||^2 \sigma^2$$

  - where $\mathbf{h}(x_0) = x_0(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$

Assessing EPE

- Earlier, we noted that the training err

$$\text{err} = \frac{1}{n}\sum_{i=1}^{n} L(y_i, \hat{f}(x_i))$$

would not typically be a good estimate of EPE

- In particular, we would expect err to be somewhat lower than the true EPE
  - that is, the estimate would be overly optimistic

- Part of the discrepancy is due to where the evaluation points occur
  - EPE refers to expected error on an independent sample
  - referred to as *extra-sample* error

Assessing EPE

- Methods that directly estimate the extra-sample error include cross-validation and the bootstrap
  - both involve the clever use and re-use of the training data
- Towards an analytic treatment of understanding the nature of the optimism associated with using the training data to evaluate generalization error, we can consider the *in-sample* error

$$\text{Err} = \frac{1}{n}\sum_{i=1}^{n} \text{E}_y\left[\text{E}_{Y^{\text{new}}}\left[L(Y_i^{\text{new}}, \hat{f}(x_i)\right]\right]$$

- The notation Y^{new} indicates that we observe n new outcome values *at each of the training points* x_i, $i = 1, \ldots, n$

Assessing EPE

- Each of the n components of the in-sample error averages over the randomness in two distributions
  - the randomness in the observed outcomes in the training data, **y**
  - the randomness in the 'new' outcome observation, Y_i^{new}
- The *optimism* is defined as the expected difference between the in-sample error and the training error

$$\text{op} \equiv \text{Err} - \text{E}_y[\text{err}]$$

  - expectation is taken with respect to the sampling distribution based on the training data, **y**

Assessing EPE

- For squared error loss, a little algebra leads to

$$\text{op} = \frac{2}{n}\sum_{i=1}^{n}\text{Cov}[\hat{y}_i, y_i]$$

Assessing EPE

- This definition leads to the relation

$$\text{Err} = \text{E}_y[\text{err}] + \frac{2}{n}\sum_{i=1}^{n}\text{Cov}[\hat{y}_i, y_i]$$

- So, the extent to which err is optimistic, as an estimator of Err, depends on how strongly y_i influences its own prediction

Assessing EPE

- The expression simplifies if $\hat{y}_i$ is linear in the y's

$$\hat{y}_i = \sum_{j=1}^{n} \pi_j y_j$$

so that

$$\begin{aligned} \text{op} &= \frac{2}{n} \sum_{i=1}^{n} \mathrm{E}_y \left[(\hat{y}_i - \mathrm{E}_y[\hat{y}_i])(y_i - \mathrm{E}_y[y_i]) \right] \\ &= \frac{2}{n} \sum_{i=1}^{n} \pi_i \mathrm{Var}[y_i] \end{aligned}$$

Assessing EPE

- For example, under the additive error model

$$Y = f(X) + \epsilon$$

with $\mathrm{E}[\epsilon] = 0$ and $\mathrm{Var}[\epsilon] = \sigma^2$, we obtain

$$\mathrm{Err} = \mathrm{E}_y[\mathrm{err}] + \frac{2}{n} p \sigma^2$$

  - p is the number of parameters fit in the regression

Estimation of in-sample error

- While decision theory tells us that EPE is a natural criterion for model selection, the in-sample error can still be useful
  - having an analytic treatment makes the approach convenient
  - can be effective if we focus on relative differences in error between model options, rather than the absolute error itself

- From the previous relation, the general form of an estimator for Err is

$$\widehat{\text{Err}} = \text{err} + \widehat{\text{op}}$$

where $\widehat{\text{op}}$ is an estimate of the optimism

Estimation of in-sample error

Mallow's C_p

- For the linear model, squared error loss leads to Mallow's C_p statistic:

$$\begin{aligned} C_p &= \text{err} + \frac{2}{n} p \sigma^2 \\ &= \frac{1}{n} \left\{ \text{RSS} + 2p\hat{\sigma}^2 \right\} \end{aligned}$$

- The estimate $\hat{\sigma}^2$ is typically taken from a low-bias model
  - the most complex model under consideration
- The C_p statistic penalizes the residual sum of squares by a factor proportional to the number of parameters being estimated
  - the more complex the model, the greater p will be and the greater the penalty

Estimation of in-sample error

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Akaike information criterion; AIC

- The Akaike information criterion is a more general estimate of Err when a log-likelihood function is used as the loss function
  - for a model parameterized by θ, we take

$$L(Y, f_\theta(X)) \;=\; -2 \log \Pr_\theta(Y|\, X)$$

  - sometimes referred to as *cross-entropy* loss or *deviance*
  - multiplying by -2 and taking the log makes the loss for the Normal distribution match the squared error loss

- We use this loss function all the time as a means for choosing the 'best' model from our training data
  - minimizing the observed loss is maximum likelihood estimation

Estimation of in-sample error

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Akaike information criterion; AIC

- AIC relies on the following relationship

$$-2\mathrm{E}_Y\left[\log \Pr_{\hat{\theta}}(Y|\, X)\right] \approx -\frac{2}{n}\mathrm{E}_y[\text{loglike}] + 2\frac{p}{n}$$

  - this relationship holds asymptotically as $n \to \infty$
  - $\hat{\theta}$ is the maximum likelihood estimate
  - 'loglike' is the maximized log-likelihood

$$\text{loglike} = \sum_{i=1}^{n} \log \Pr_{\hat{\theta}}(y_i|\, X)$$

Estimation of in-sample error

Akaike information criterion; AIC

- For any general purpose likelihood AIC is defined as

$$\text{AIC} = -\frac{2}{n}\text{loglike} + 2\frac{p}{n}$$

  - for the Normal model, with $\hat{\sigma}^2$ known, this is equivalent to C_p

- The penalty imposed by AIC is similar to that imposed by C_p
  - proportional to the number of parameters being estimated

- In more general settings, when the estimator is linear

$$\hat{\mathbf{y}} = \mathbf{L}\mathbf{y}$$

  we can replace p with the effective degrees of freedom $\text{df} = \text{tr}(\mathbf{L})$ (eg. penalized regression methods)

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