Lecture 6

Generalization

ISLR 5, ESL 7,8

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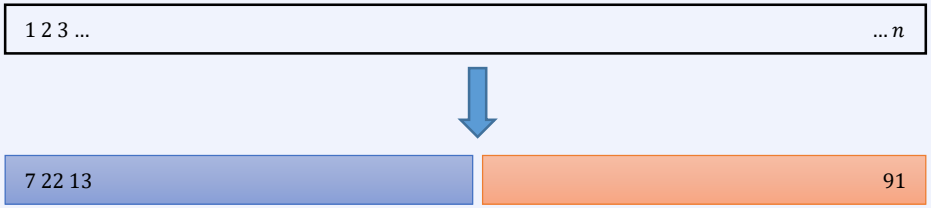
Validation

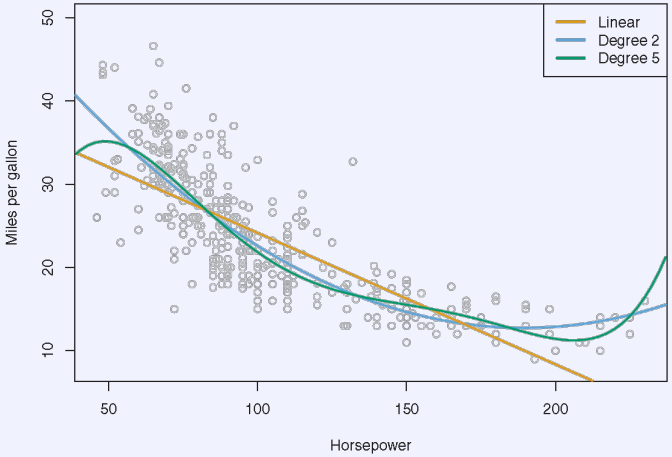
To estimate how well a model generalizes, we should test on different data than we trained on

The most basic approach is to randomly divide the data into two

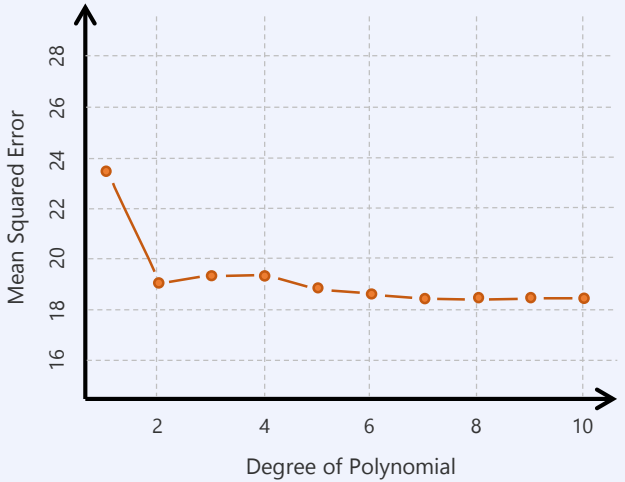
- we fit our models using the training data
- we estimate the generalization error (aka test error) on the test data (aka hold-out set)



Example Validation



$$\texttt{mpg} = \beta_0 + \beta_1 \times \texttt{horsepower} + \beta_2 \times \texttt{horsepower}^2 + \varepsilon$$



Validation error for one random 50-50 splits into training and validation set

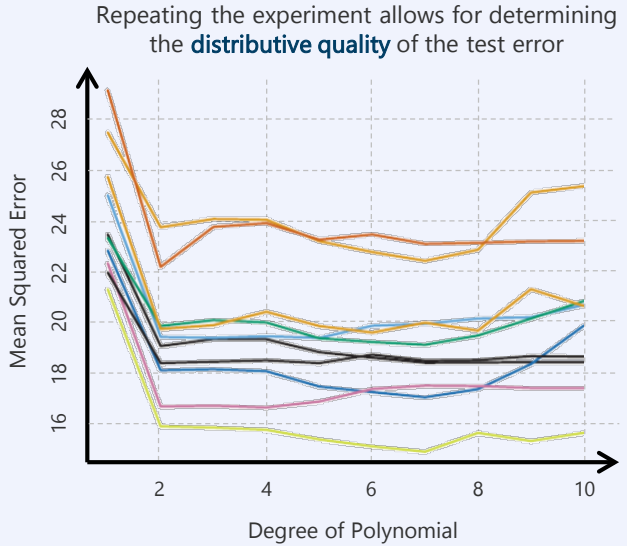
Validation Set Approach

Observations

1. test error can vary widely
2. quadratic term affords large improvement of test error
3. higher-order terms not of benefit

Problems

1. high variability of estimated test error
2. training set becomes smaller;
   model may be suboptimal (undertrained);
   test error may be overestimated

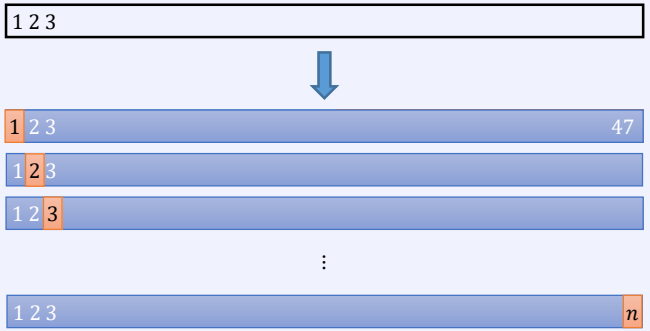


Validation error for one random 50-50 splits into training and validation set

Leave-one-out Cross Validation (LOOCV)

Key idea: set only one data point aside for testing

- training set is now as large as can be, so little bias
- but, only one point to test on, so high variance



Repeating for every data point averages out variance

$$MSE_i = (y_i - \hat{y}_i)^2$$

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

- process is deterministic, repeating always gives same result

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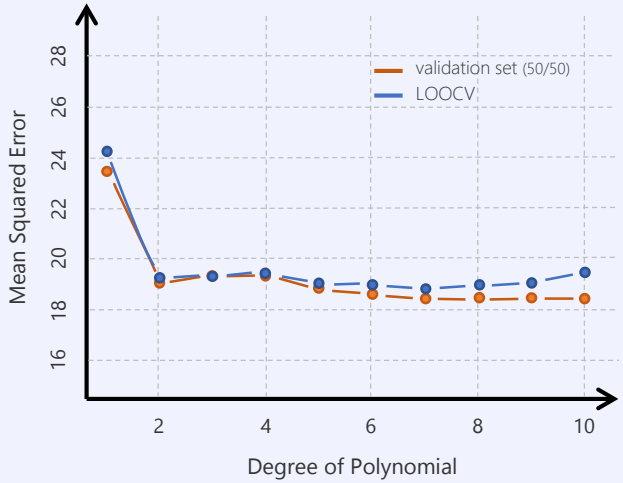
$$CV_{(n)} = \frac{1}{n}\sum_{i=1}^{n} MSE_i$$

- process is deterministic, repeating always gives same result
- for least-squares linear or polynomial regression we have

$$CV_{(n)} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \hat{y}_i}{1 - h_i}\right)^2$$



(h_i is the leverage statistic from Lecture 3)

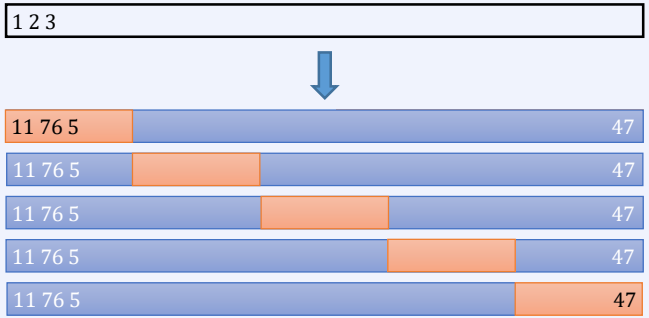
k-fold Cross Validation

Randomly divide the data into k folds

- train on $k-1$ folds, test on the remaining 1 fold
- repeat such that all folds have been tested on
- gives k estimates of the test error, the final estimate is

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

- in practice, we use $k = 5$ or 10
- LOOCV is k-fold CV with $k = n-1$
- k-fold CV is more efficient but has higher bias than LOOCV



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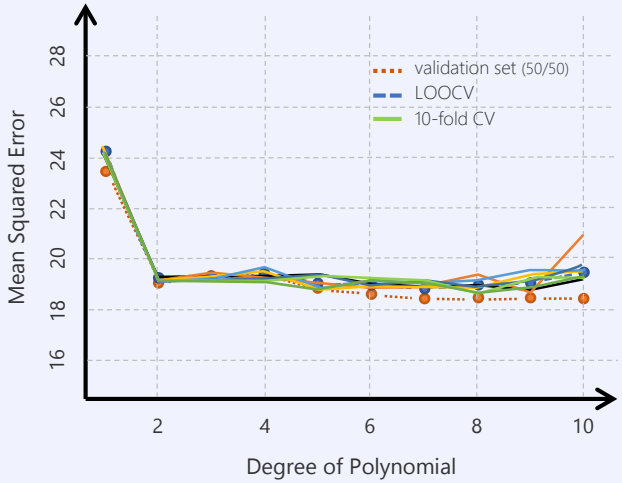
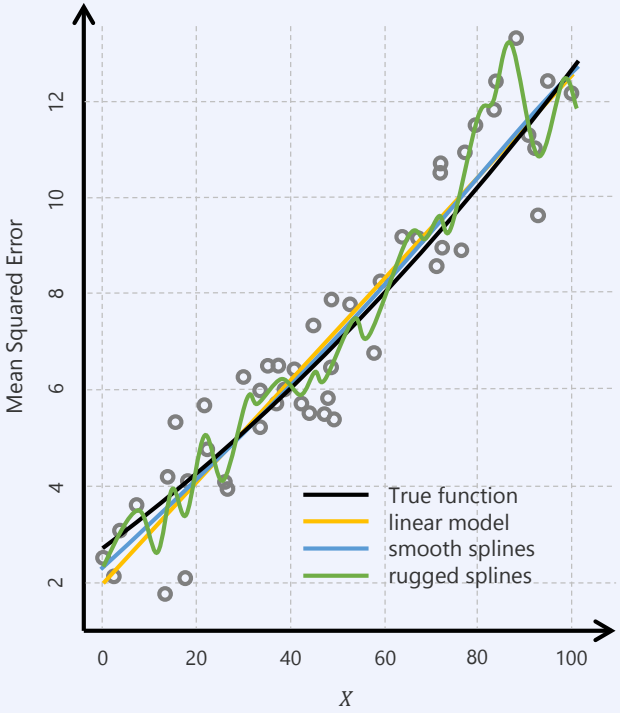
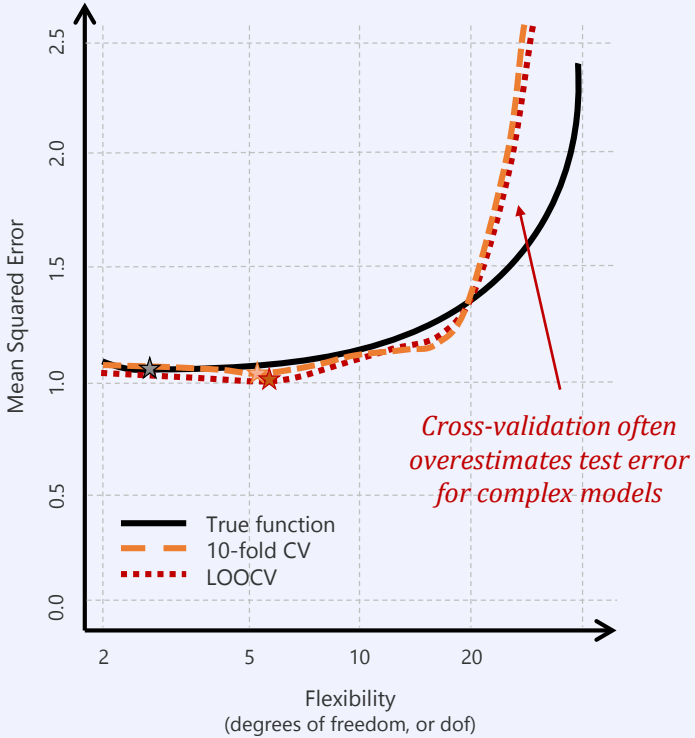
We can reduce variance of the CV-estimated error by averaging the over different (e.g. 10) random splits



10-fold cross-validation on 10 different random splits

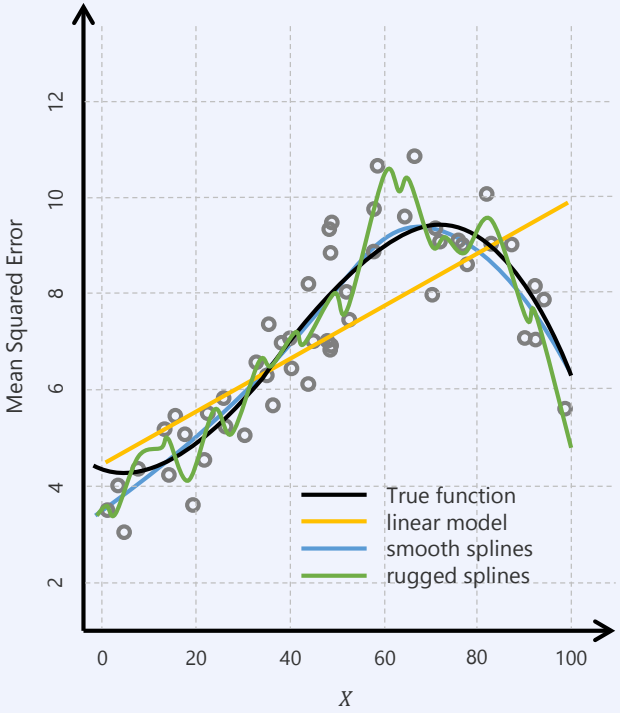
Example almost-linear data

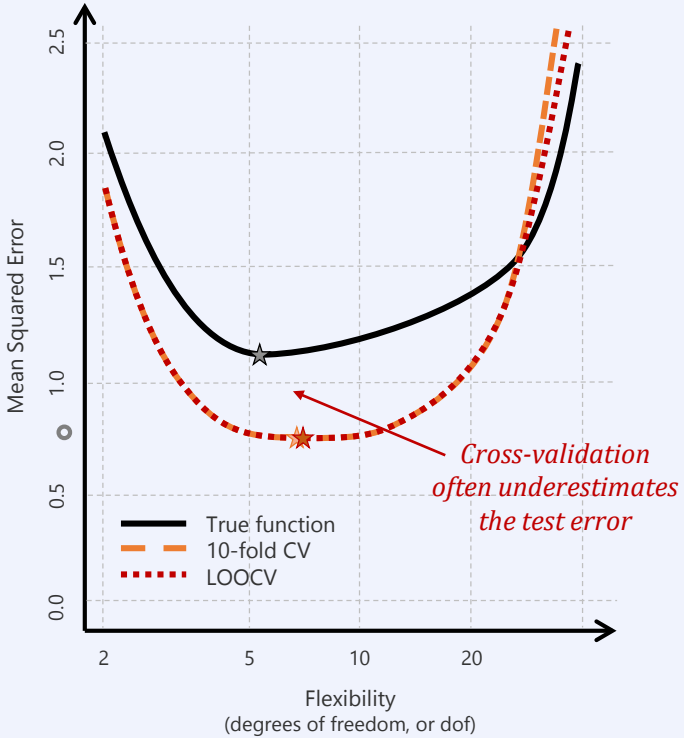




(ISL 5.1.3)

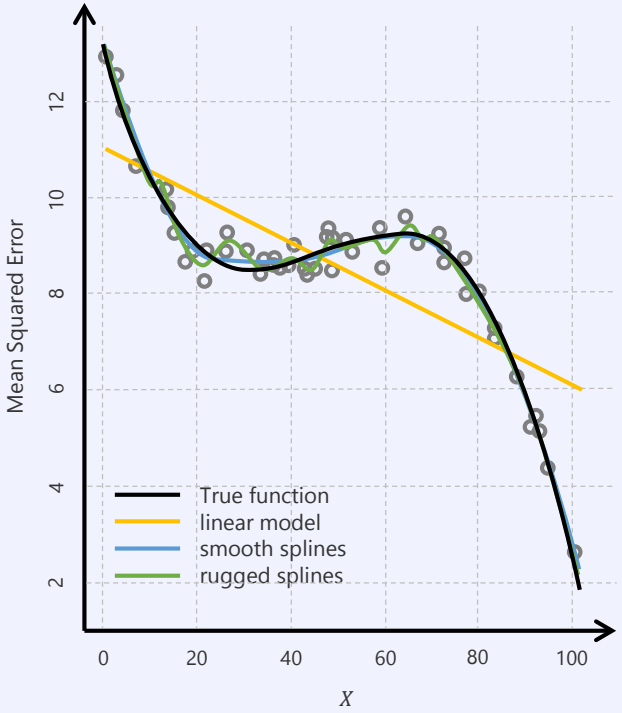
Example moderately non-linear data

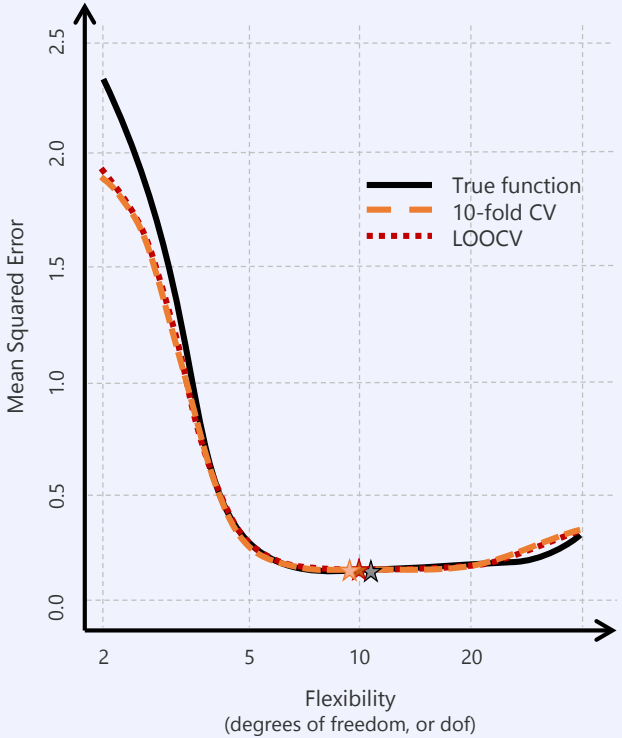




(ISL 5.1.3)

Example highly non-linear data





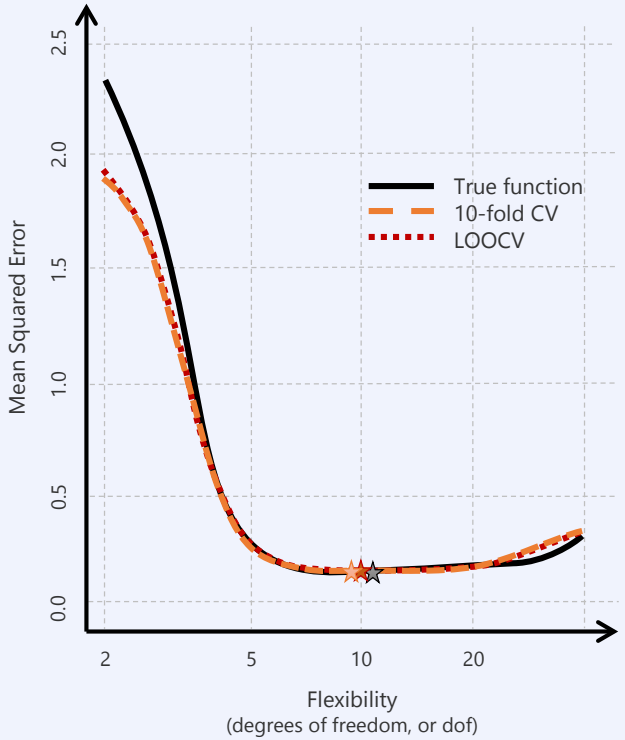
(ISL 5.1.3)

k-fold Cross Validation

We are often not only interested in
the test error itself, but even more interested in
the location of the minimum, as that shows
the complexity of the optimal model

- test errors vary so minimum is difficult to identify
- use CV to estimate variance of the test error!
- many different models have almost the same error

General rule:
Choose the simplest model within
1 standard error of the optimum



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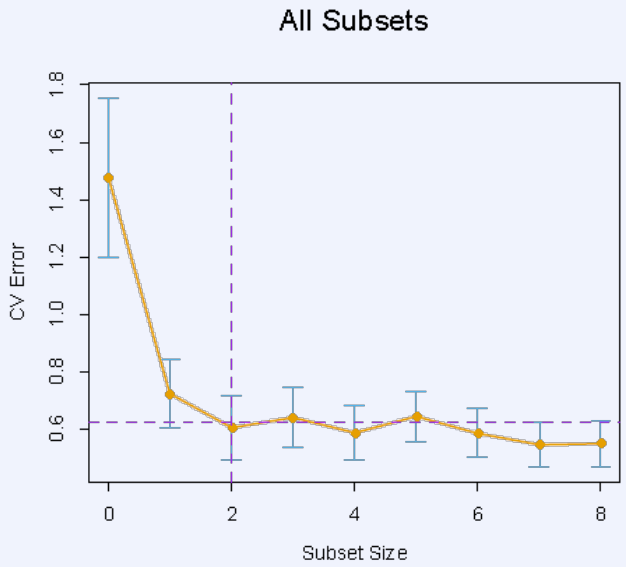


(ISL 5.1.3)

Bias-Variance Tradeoff for k-fold CV

k-fold CV often gives more accurate error estimates than LOOCV

- this is due to the bias-variance tradeoff

Increasing the relative size of the training set reduces bias but increases variance

- LOOCV averages over models trained on almost the same data: all estimates are highly correlated
- k-fold CV has less overlap in training data, and hence less correlated estimates

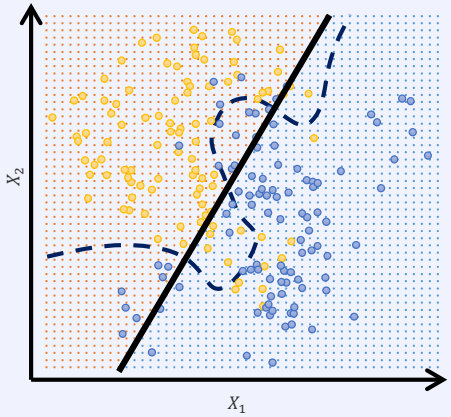
error estimates ↓ *different folds* ↓

The variance of the average over the outcomes of k identically distributed events with correlation ρ, each with variance σ^2 is

↑ *correlation between folds* ↑ *of error estimate in a fold*

$$\rho\sigma^2 + \frac{1-\rho}{k}\sigma^2$$

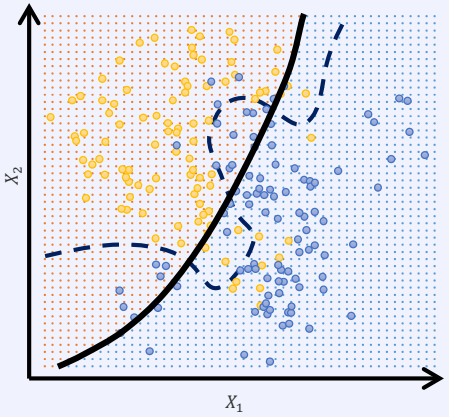
Example Cross Validation for Classification



Logistic Regression
degree = 1

$$\log\frac{p}{1-p} = \beta_0 + \beta_1 X_1 + \beta_2 X_2$$

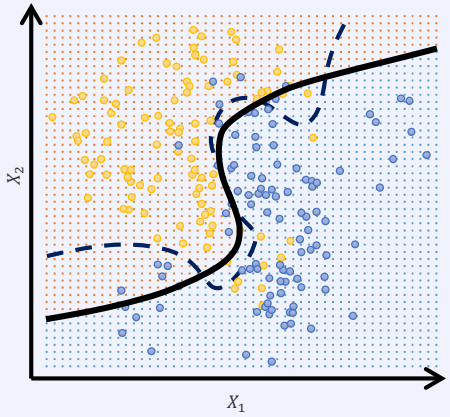
test error 0.201



Quadratic Logistic Regression
degree = 2

$$\log\frac{p}{1-p} = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_2 + \beta_4 X_2^2$$

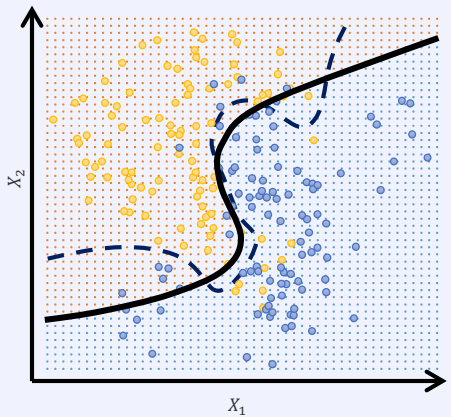
test error 0.197



Qubic Logistic Regression
degree = 3

$$\log\frac{p}{1-p} = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_1^3 + \cdots$$

test error 0.160



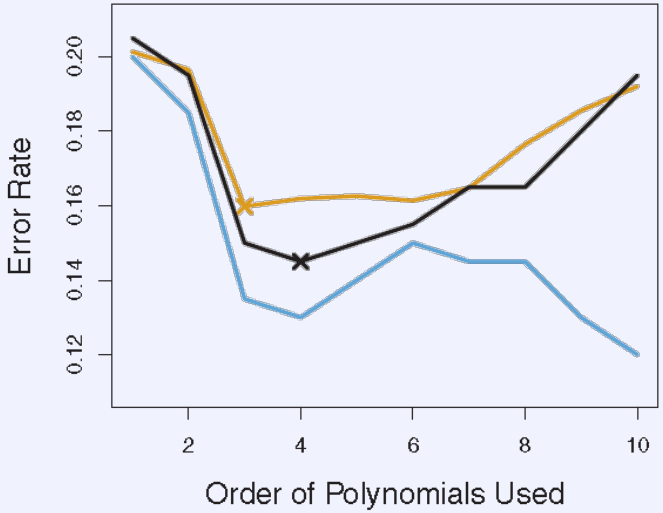
Quartic Logistic Regression
degree = 4

$$\log\frac{p}{1-p} = \beta_0 + \beta_1 X_1 + \beta_2 X_1^2 + \beta_3 X_1^3 + \beta_4 X_1^4 + \cdots$$

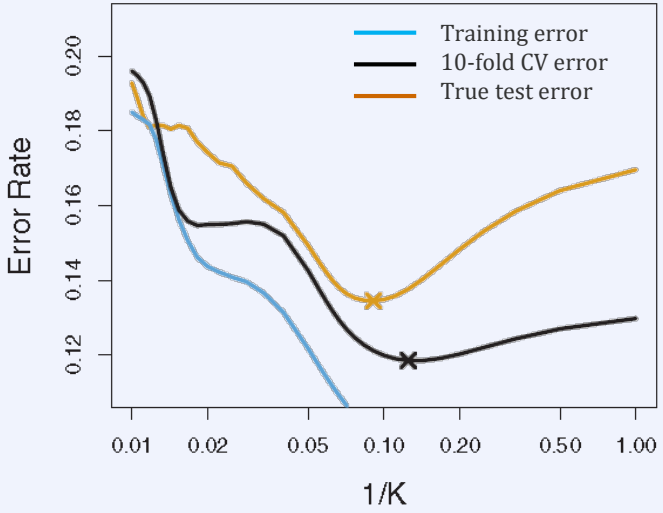
test error 0.162

Test error (true) for Logistic Regression on synthetic data
(Bayes error 0.11)

Example Cross Validation for Classification



CV estimates of test error
logistic regression



CV estimates of test error
k-NN classification

Doing Cross Validation ~~Right~~ Wrong

Assume a scenario with many predictors

How we typically build a model

1. select the predictors with strongest univariate correlation with the output
2. build a multivariate model on these predictors
3. use CV to select the model parameters

Now, let's assume we get

- $N = 50$ samples, two balanced classes
- $p = 5000$ continuous-valued Gaussian predictors, independent of class labels

The true test error of any classifier is 50%

Let's build that model!

1. select 100 predictors in step 1
2. use $\mathbf{1}$-NN classifier on these predictors
3. do CV in 50 simulations to estimate test error

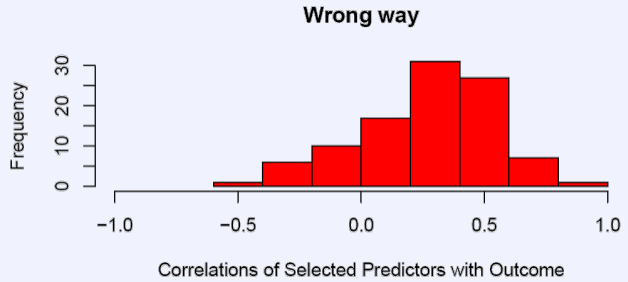
Resulting average test error is 3%

- what? how? why? what is this? I don't even?
- the predictors we chose have an unfair advantage, as we chose them over all data, rather than over just the training data
- Always keep training and test set separate!

Doing Cross Validation Wrong

The Wrong Way

1. select the 100 predictors most correlated with the outcome variable using all n samples
2. choose a random set of 10 samples
3. compute correlations of selected predictors with the output over just these 10 samples



Mean correlation of selected predictors with outcome is 28%

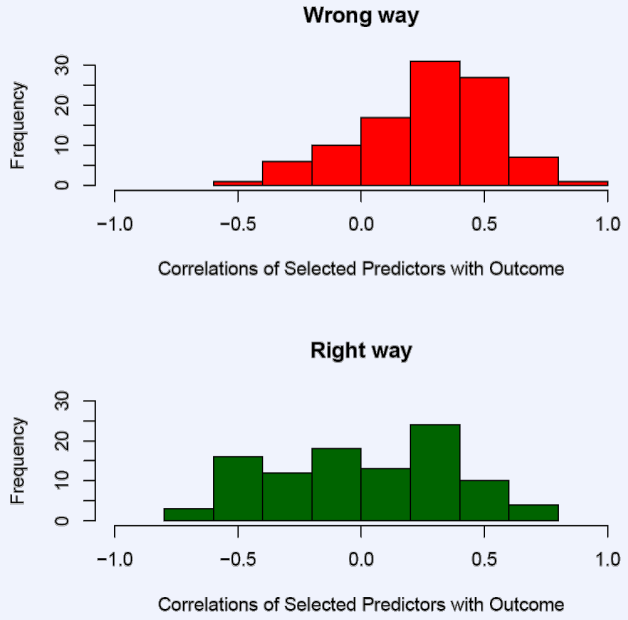
Doing Cross Validation Right

The Right Way

1. divide samples into K classes (K-fold CV)
2. for each k=1,..., K do
    1. find that subset of predictors most correlated with the outcome on all samples except those in fold k
    2. use these predictors to build multivariate model
    3. use classifier to predict classes of samples in fold k
3. accumulate errors on all K folds to compute correlation

In a multistep procedure, we have to apply cross-validation to entire sequence of steps!

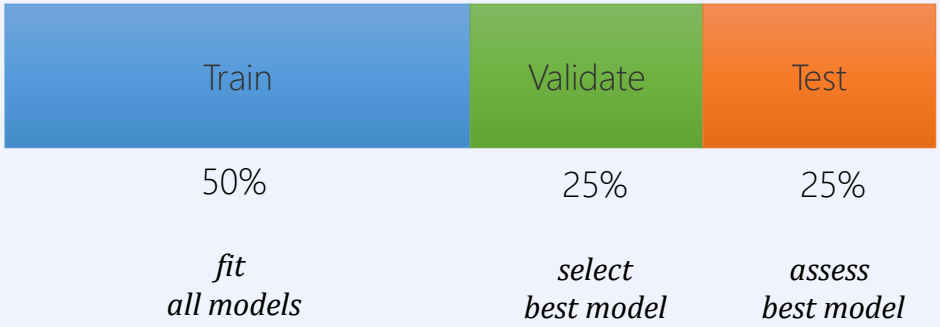
- initial clustering can be done before samples are left out (because it does not use class labels), e.g. select 50 predictors with highest variances across the training set



Train-Validation-Test Paradigm

More conservatively, we can divide the data three-way

1. training set for fitting models
2. validation set for comparatively assessing model performance in order to select a model
3. test set in order to assess the performance of the selected model



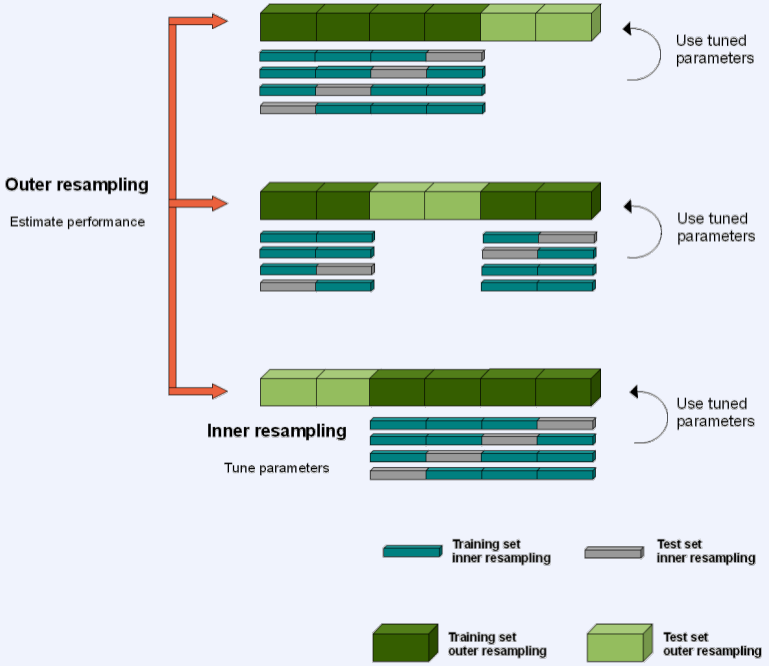
Nested Cross Validation

Purpose: optimize hyper-parameters first, then assess performance of the best model

- **inner cross validation** for tuning hyper-parameters and model selection
- **outer cross validation** for evaluating performance of the final model

Provides more conservative error estimates than normal cross-validation

- different test sets for selecting model parameters and assessing model performance



(https://mlr-org.github.io/mlr-tutorial/devel/html/nested_resampling/index.html)

The Bootstrap

ISLR 5.2, ESL 7.11

The Bootstrap

Bootstrap is used to quantify the uncertainty of a given estimator

- for linear least-squares regression, we already saw theoretical methods (and software) for doing so
- the bootstrap is applicable to all kinds of methods for which no theory exists

Toy example

- we want to invest a fixed sum in two assets that yield returns X and Y, fraction α in X and $1-\alpha$ in Y
- we want to choose α such that we minimize the total risk (variance) of the investment $\mathrm{Var}(\alpha X + (1-\alpha)Y)$

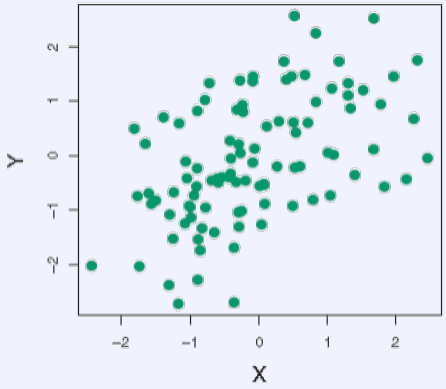
$$\alpha = \frac{\sigma_Y^2 - \sigma_{XY}}{\sigma_X^2 + \sigma_Y^2 - 2\sigma_{XY}}$$

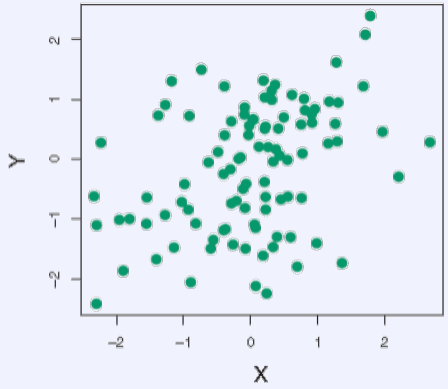
$$\sigma_X^2 = \mathrm{Var}(X) \qquad \sigma_Y^2 = \mathrm{Var}(Y) \qquad \sigma_{XY} = \mathrm{Cov}(X, Y)$$

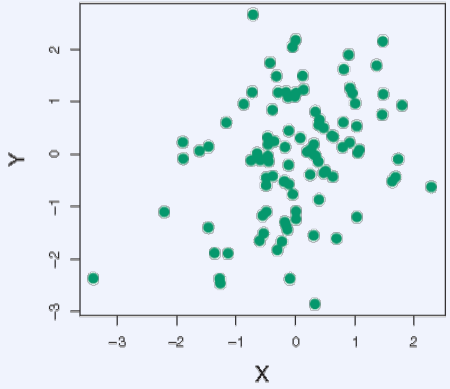
- our estimate of α will hence depend on the sample estimates of the variances

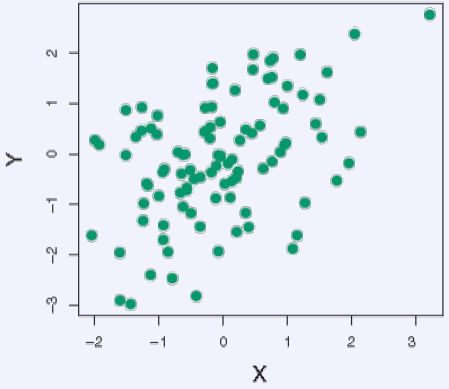
$$\hat{\alpha} = \frac{\hat{\sigma}_Y^2 - \hat{\sigma}_{XY}}{\hat{\sigma}_X^2 + \hat{\sigma}_Y^2 - 2\hat{\sigma}_{XY}}$$

The Bootstrap









What are the estimates of α when we *repeatedly* draw 100 samples?

The Bootstrap

We repeat the process 1000 times, obtaining estimates $\alpha_1, \alpha_2, \ldots, \alpha_{1000}$

$$\bar{\alpha} = \frac{1}{1{,}000} \sum_{r=1}^{1{,}000} \hat{\alpha}_r = 0.5996$$

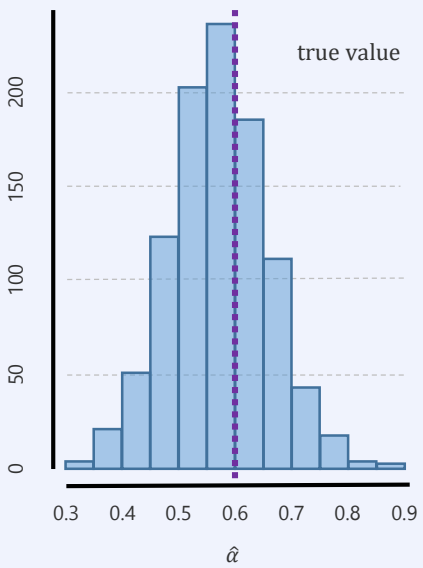
$$SE(\hat{\alpha}) = \sqrt{\frac{1}{1{,}000 - 1} \sum_{r=1}^{1{,}000} (\hat{\alpha}_r - \alpha)^2} = 0.083$$

In a real setting, we cannot get new samples

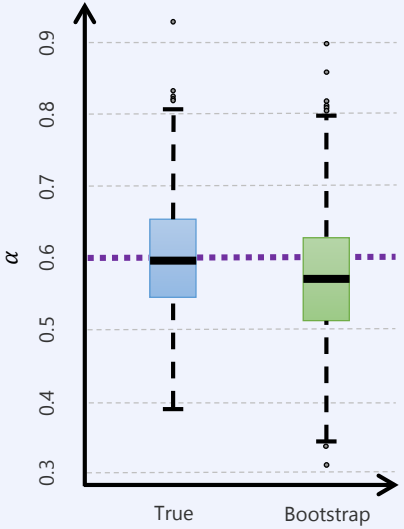
- but, we can re-sample from the training data
- we draw uniformly and with replacement $B = 1000$ samples Z^{*i} each of size n
- then

$$SE_{B(\hat{\alpha})} = \sqrt{\frac{1}{B-1} \sum_{r=1}^{B} \left(\hat{\alpha}^{*r} - \frac{1}{B} \sum_{r'=1}^{B} \hat{\alpha}^{*r'} \right)^2}$$

Thousand estimates of α



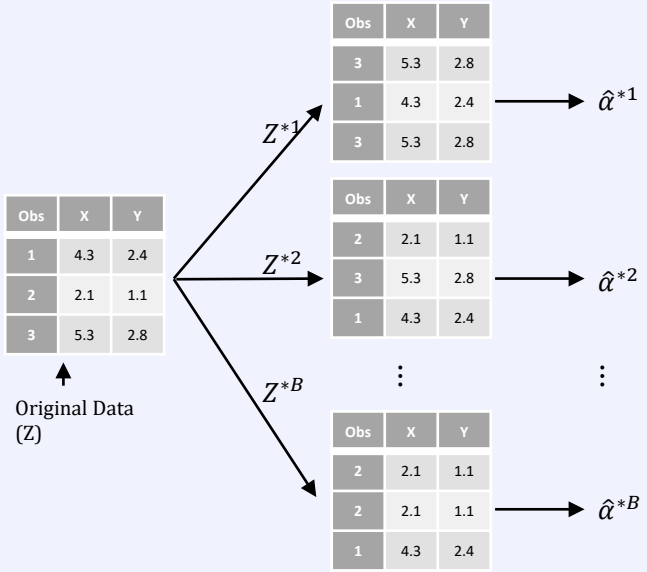
Simulated data vs. Bootstrap



$\sigma_X^2 = 1$
$\sigma_Y^2 = 1.25$
$\sigma_{XY} = 0.5$
$\alpha = 0.6$

$\hat{\alpha} = 0.5996$
$SE(\hat{\alpha}) = 0.083$

Example The Bootstrap



Bootstrap on a data set of 3 rows

The Bootstrap

Bootstrap samples tend to contain only a subset of the training data

- some of the training observations will occur multiple times in a bootstrap set
- we have compute the probability of an observation being selected into a bootstrap set as

$$\Pr\{\text{observation } i \in \text{bootstrap sample } b\} = 1 - \left(1 - \frac{1}{n}\right)^n \approx 1 - e^{-1} = 0.632$$

On average, about a third of the data is not contained in a bootstrap sample

- we should test the model on these out-of-bag samples, mimicking 3-fold CV
- if we *do include* in-bag samples, training and test set overlap, and we will underestimate the test error

Bootstrap samples are highly correlated, which increases the variance of the error estimate

Conclusion for today

To estimate how well a model generalizes, we have to test on *other* data than it was trained on

Resampling or subsampling are methods for repeatedly drawing samples from training data to

- learn about the variability of the fitted models, as the training set changes (model variability)
- assess the test error which is hard to estimate (model assessment)
- optimize model performance in terms of test error (model selection)

Resampling methods can be computationally expensive

- repeated model fitting on a potentially large number of data sets
- today's computing power allows for this expense
- but not when your model is extremely expensive (looking at you, Deep Learning)