Chapter 7: Model Assessment and Selection

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April 20, 2012

Introduction

Regression: Review of our problem

- Have target variable Y to estimate from a vector of inputs X.
- A prediction model $\hat{f}(X)$ has been estimated from training data $\mathcal{T} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$.
- The loss function $L(Y, \hat{f}(X))$ measures the errors between Y and $\hat{f}(X)$.
- Common loss functions are

$$L(Y, \hat{f}(X)) = \begin{cases} (Y - \hat{f}(X))^2 & \textbf{squared error}, \\ |Y - \hat{f}(X)| & \textbf{absolute error} \end{cases}$$

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Definition of **Test Error**

Test Error a.k.a. **generalization error**

$$\boxed{\mathsf{Err}_{\mathcal{T}} = E[\, L(Y, \hat{f}(X)) \,|\, \mathcal{T} \,]}$$

- Prediction error over an independent test sample.
- X and Y are drawn randomly from $p(X, Y)$.
- The training set $\mathcal{T}$ if fixed.

Definition of **Expected Prediction Error**

Expected Prediction Error (expected test error)

$$\boxed{\text{Err} = E[\,L(Y, \hat{f}(X))\,] = E[\,\text{Err}_{\mathcal{T}}\,]}$$

- In this case take expectation over all the random quantities including the training set.

Which quantities interest us

- Would like to estimate $\text{Err}_{\mathcal{T}}$.
- But in most cases it is easier to estimate Err. Why??

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Definition of **Training Error**

Training error

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

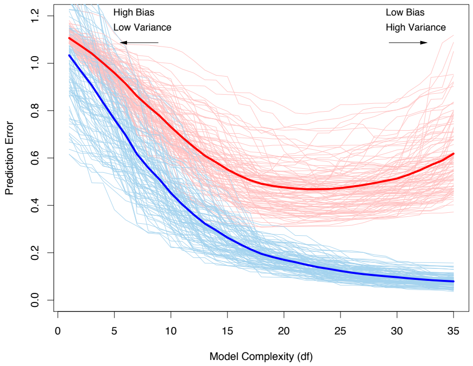
Already know as complexity of $\hat{f}$ increases

- then $\overline{\text{err}} \to 0$,
- but there is a tendency to overfit and $\text{Err}_{\mathcal{T}}$ increases
- $\overline{\text{err}}$ is not a good estimate of $\text{Err}_{\mathcal{T}}$ or Err.

We will be revisiting the **Bias-Variance** trade-off.

Issues in assessing generalization ability

Test and training error as model complexity increases.



1. Light blue curve: training error $\overline{\text{err}}$.
2. Solid blue curve: expected training error $E[\overline{\text{err}}]$.
3. Light red curve: conditional test error $\text{Err}_{\mathcal{T}}$.
4. Solid red curve: expected test error Err.

Same story for classification

- Have target categorical variable $G \in \{1, \dots, K\}$ to estimate from a vector of inputs X.
- Typically model $p_k(X) = P(G = k|X)$ and define

$$\hat{G}(X) = \arg\max_k p_k(X)$$

- Common loss functions are
  1. **0-1 loss**

$$L(G, \hat{G}(X)) = \text{Ind}(G \neq \hat{G}(X))$$

  2. **log-likelihood** a.ka. deviance

$$L(G, \hat{p}(X)) = -2 \sum_{k=1}^{K} \text{Ind}(G = k)\, \hat{p}_k(X) = -2\, \log \hat{p}_G(X)$$

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Performance scores for classification

- **Test Error**

$$\boxed{\mathsf{Err}_{\mathcal{T}} = E[\, L(G, \hat{G}(X)) \,|\, \mathcal{T}\,]}$$

- **Training Error** one common definition

$$\boxed{\overline{\mathsf{err}} = -\frac{2}{n} \sum_{i=1}^{n} \log \hat{p}_{g_i}(x_i)}$$

Goal of this chapter

- $\hat{f}_\alpha(x)$ typically has a tunable parameter α controlling its complexity.

- Want to find the value of α s.t.

$$\boxed{\hat{\alpha} = \arg\min_{\alpha} E[\, L(Y, \hat{f}_\alpha(X)) \,]}$$

- Estimate $E[\, L(Y, \hat{f}_\alpha(X)) \,]$ for different values of α.

- This chapter presents methods how to do this.

- Choose the α with minimum estimate.

Our two separate goals

Model selection

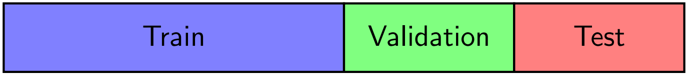
Estimate the performance of different models in order to choose the best one.

Model Assessment

Having chosen a final model, estimate its prediction error on new data.

For a data-rich situation

Randomly divide the dataset into 3 parts



Common split ratio 50%, 25%, 25%.

Model Selection

- Use **training set** to fit each model.
- Use **validation set** to estimate $\text{Err}_{\mathcal{T}}$ for each model.
- Choose model with lowest $\text{Err}_{\mathcal{T}}$ estimate.

Model Assessment of the chosen model

- Use the **test set** - unseen until this stage - to estimate $\text{Err}_{\mathcal{T}}$.

What if labelled data-sets are small ?

Approximate the **validation step** either

- analytically with approaches such as
  1. Akaike Information Criterion
  2. Baysian Information Criterion
  3. Minimum Description Length
  4. Structural Risk Minimization

  or

- with efficient sample re-use
  1. cross-validation
  2. the bootstrap

Each method also provides estimates of Err or $\text{Err}_{\mathcal{T}}$ of the final chosen model.

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The Bias-Variance Decomposition

The bias-variance decomposition

- Will assume an additive model

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

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

- Then the **expected prediction error** of $\hat{f}(X)$ at $X = x_0$

$$\mathrm{Err}(x_0) = \mathrm{E}[(Y - \hat{f}(x_0))^2 | X = x_0]$$

can be expressed as

$$\boxed{\mathrm{Err}(x_0) = \text{Irreducible Error} + \text{Bias}^2 + \text{Variance}}$$

Irreducible error:	σ_ϵ^2,
Bias:	$\mathrm{E}[\hat{f}(x_0) - f(x_0)]$,
Variance:	$\mathrm{Var}[\hat{f}(x_0)]$

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k-nearest neighbour regression fit

$$\boxed{\text{Err}(x_0) = \sigma_\epsilon^2 + \underbrace{\left[f(x_0) - \frac{1}{k}\sum_{l=1}^{k} f(x_{(l)}) \right]^2}_{\text{squared bias}} + \underbrace{\frac{\sigma_\epsilon^2}{k}}_{\text{variance}}}$$

- Complexity of model is inversely related k.
- As k increases the variance decreases.
- As k increases the squared bias increases.

The above expression was computed by assuming the x_i's are fixed.

Linear model - least square fit

Have a linear model

$$\hat{f}_p(x) = x^t \hat{\beta}$$

where $\hat{\beta}$ is p-dimensional and fit by least squares, then

$$\boxed{\text{Err}(x_0) = \sigma_\epsilon^2 + \left[f(x_0) - E[\,\hat{f}_p(x_0)\,] \right]^2 + \|h(x_0)\|^2 \, \sigma_\epsilon^2}$$

with $h(x_0) = \mathbf{X}(\mathbf{X}^t\mathbf{X})^{-1} x_0$ and $\hat{f}_p(x_0) = x_0^t(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t y$.

Linear model - ridge regression fit

Have a linear model

$$\hat{f}_{p,\alpha}(x) = x^t \hat{\beta}_\alpha$$

where $\hat{\beta}_\alpha$ is p-dimensional and fit via ridge regression, then

$$\boxed{\text{Err}(x_0) = \sigma_\epsilon^2 + \left[f(x_0) - E[\,\hat{f}_{p,\alpha}(x_0)\,]\right]^2 + \|h_\alpha(x_0)\|^2\,\sigma_\epsilon^2}$$

with

$$h_\alpha(x_0) = \mathbf{X}(\mathbf{X}^t\mathbf{X} + \alpha I)^{-1} x_0$$

$$\hat{f}_{p,\alpha}(x_0) = x_0^t(\mathbf{X}^t\mathbf{X} + \alpha I)^{-1}\mathbf{X}^t\, y$$

Therefore this regression fit model has a different bias and variance to the least square fit.

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Therefore this regression fit model has a different bias and variance to the least square fit.

Linear model - Finer decomposition of the bias

Let β_* denote the parameters of the best-fitting linear approx to f:

$$\beta_* = \arg\min_{\beta} E[\,(f(X) - X^t\beta)^2\,]$$

Can write the **averaged squared bias**

$$E_{x_0}\left[(f(x_0) - E[\,\hat{f}_\alpha(x_0)\,])^2\right]$$

as

$$\boxed{\underbrace{E_{x_0}[\,(f(x_0) - x_0^t\beta_*)^2\,]}_{\text{Ave[Model Bias]}^2} + \underbrace{E_{x_0}[\,(x_0^t\beta_* - E[x_0^t\hat{\beta}_\alpha])^2\,]}_{\text{Ave[Estimation Bias]}^2}}$$

- Estimation bias is zero for ordinary least sq. estimate.
- Estimation bias is positive for ridge regression estimate.

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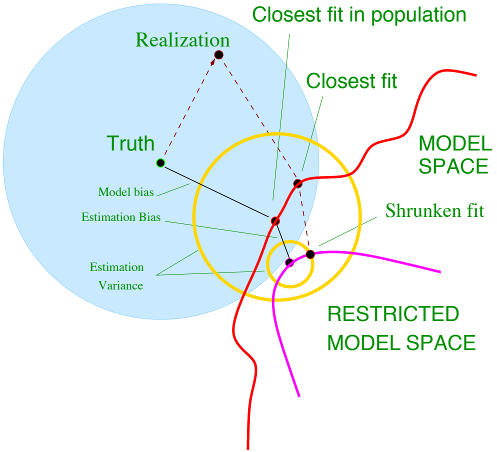
Behaviour of bias and variance



Bias-variance trade-off: Example 1

The Set-up

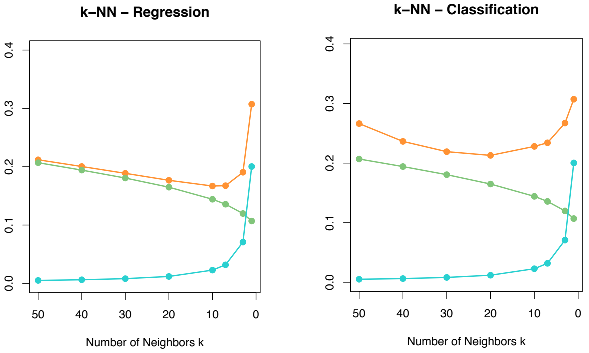
- Have $n = 80$ observations and $p = 20$ predictors.
- X is uniformly distributed in $[0, 1]^{20}$ and

$$Y = \begin{cases} 0 & \text{if } X_1 \le .5 \\ 1 & \text{if } X_1 > .5 \end{cases}$$

- Apply k-nn to perform both the classification and regression tasks.
- Use **squared error loss** to measure **Err** for the **regression task**.
- Use **0-1 loss** to measure **Err** for the **classification task**.

Bias-variance trade-off: Example 1

Expected prediction error as k varies



- Orange curve: **expected prediction error**
- Green curve: **squared bias**
- Blue curve: **variance**

Note prediction error curves are not the same as the loss functions differ.

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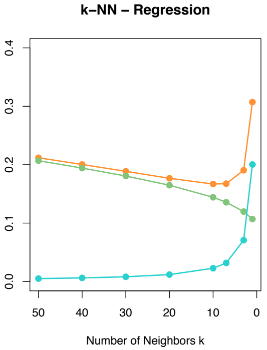

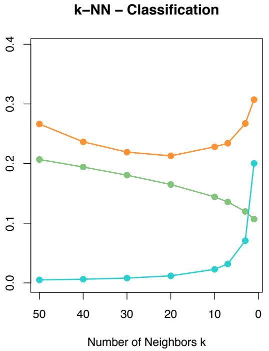

- Orange curve: **expected prediction error**
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Bias-variance trade-off: Example 2

The Set-up

- Have $n = 80$ observations and $p = 20$ predictors.
- X is uniformly distributed in $[0,1]^{20}$ and

$$Y = \begin{cases} 1 & \text{if } \sum_{j=1}^{10} X_j > 5 \\ 0 & \text{otherwise} \end{cases}$$

- Use best subset linear regression of size p for classification and regression tasks.
- Use **squared error loss** to measure **Err** for the **regression task**.
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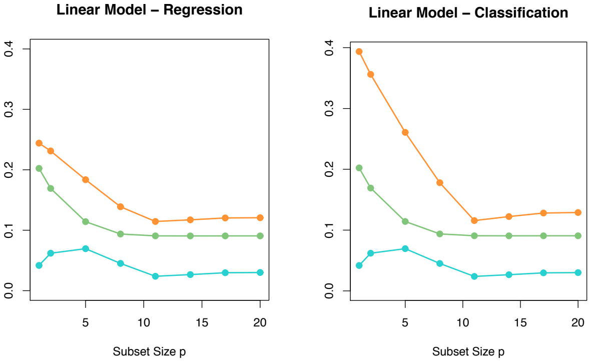
Bias-variance trade-off: Example 2

Expected prediction error as p varies



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Optimism of the Training Error Rate

Estimating the optimism of $\overline{\text{err}}$

- Training error $\overline{\text{err}} \ll \text{Err}_{\mathcal{T}}$ as it uses $\mathcal{T}$ for both fitting and assessment.

- **One factor is**

  The training and test input vectors

  - for $\overline{\text{err}}$ are the same.
  - while for $\text{Err}_{\mathcal{T}}$ they differ.

- Can begin to understand the optimism of $\overline{\text{err}}$ if we focus on **in-sample error**

$$\text{Err}_{\text{in}} = \frac{1}{n} \sum_{i=1}^{n} E_{Y'}[\, L(y_i', \hat{f}(x_i)) | \mathcal{T}\,]$$

  where expectation is over new responses y_i' at each training point x_i.

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The optimism of $\overline{\text{err}}$

- Define the **optimism** as

$$\boxed{\text{op} = \text{Err}_{\text{in}} - \overline{\text{err}}}$$

- The **average optimism** is

$$\boxed{\omega = \text{E}_{\mathbf{y}}[\text{op}]}$$

where

  - the training input vectors are held fixed,
  - the expectation is over the training output values.

- For many loss functions

$$\boxed{\omega = \frac{1}{n}\sum_{i=1}^{n} \text{Cov}(\hat{y}_i, y_i)}$$

The optimism of $\overline{\text{err}}$

$$\boxed{\omega = \frac{1}{n}\sum_{i=1}^{n} \text{Cov}(\hat{y}_i, y_i)}$$

- The more strongly y_i affects its prediction $\hat{y}_i$ the larger ω.
- The larger ω the greater the optimism of $\overline{\text{err}}$.
- In summary get the important relation

$$\boxed{\text{E}_{\mathbf{y}}[\text{Err}_{\text{in}}] = \text{E}_{\mathbf{y}}[\overline{\text{err}}] + \frac{1}{n}\sum_{i=1}^{n} \text{Cov}(\hat{y}_i, y_i)}$$

How to estimate prediction error?

Option 1

- Estimate the optimism and add it to $\overline{\text{err}}$
- The methods $C_p, \text{AIC}, \text{BIC}$ work in this way for a special class estimates.
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Option 2

- Use cross-validation and bootstrap as direct estimates of the **extra-sample** Err.

Estimates of In-Sample Prediction Error

Err_{in} estimate: C_p statistic

- If $\hat{y}_i$ is obtained by a linear fit with d inputs then

$$\sum_{i=1}^{n} \text{Cov}(\hat{y}_i, y_i) = d\,\sigma_\epsilon^2$$

for the additive error model $Y = f(X) + \epsilon$.

- And so

$$\boxed{\text{E}_{\mathbf{y}}[\text{Err}_{\text{in}}] = \text{E}_{\mathbf{y}}[\overline{\text{err}}] + 2\,\frac{d}{n}\sigma_\epsilon^2}$$

- Adapting this expression leads to the C_p statistic

$$\boxed{C_p = \overline{\text{err}} + 2\,\frac{d}{n}\hat{\sigma}_\epsilon^2}$$

where $\hat{\sigma}_\epsilon^2$ is an estimate of the noise variance.

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Akaike Information Criterion

$$\boxed{\text{AIC} = \overset{\text{rewards the fit between the model and the data}}{-\frac{2}{n}\text{loglik}} + \underset{\text{penalty for including extra predictors in the model}}{2\frac{d}{n}}}$$

where

$$\text{loglik} = \sum_{i=1}^{n} \log P_{\hat{\theta}}(y_i)$$

and $\hat{\theta}$ is the MLE of θ.

Note: AIC can be seen as an estimate of $\mathrm{Err}_{\mathsf{in}}$ in this case with a log-likelihood loss.

Akaike Information Criterion: using training error

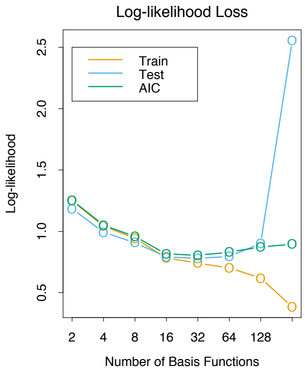
- Have a set of models $f_\alpha(x)$ indexed by α,
- $\overline{\text{err}}$ is the training error,
- $d(\alpha)$ the # of parameters for each model.

then

$$\boxed{\text{AIC}(\alpha) = \overline{\text{err}}(\alpha) + 2\frac{d(\alpha)}{n}\hat{\sigma}_\epsilon^2}$$

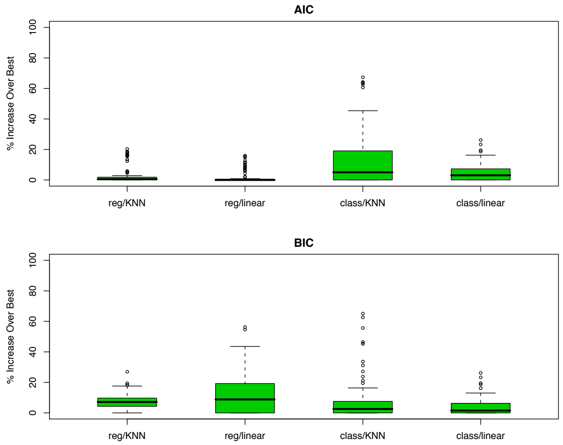
Note: AIC can be seen as an estimate of Err_{in} in this case with a squared-error loss.

AIC used for model selection



- Classifier is a logistic regression function with an expansion of M spline basis functions.
- AIC is used to estimate Err_{in} with a log-likelihood loss,
- AIC does well except when $M = 256$ is large and $n = 1000$.

How well AIC and BIC perform wrt model selection



- Boxplots show $100 \frac{\text{Err}(\hat{\alpha}) - \min_\alpha \text{Err}(\alpha)}{\max_\alpha \text{Err}(\alpha) - \min_\alpha \text{Err}(\alpha)}$ where $\hat{\alpha}$ is the best parameter found via the selection method under investigation.
- 100 training sets were used.

The Effective Number of Parameters

Generalization of the *number of parameters*

- For **regularized fitting** need to generalize the concept of *number of parameters*.
- Consider regularized linear fitting - ridge regression, cubic smoothing splines

$$\boxed{\hat{y} = \mathbf{S}\, y}$$

where

1. $y = (y_1, y_2, \ldots, y_n)^t$ is the vector of training outputs,
2. $\hat{y} = (\hat{y}_1, \ldots, \hat{y}_n)$ is the vector of predictions,
3. $\mathbf{S}$ is an $n \times n$ matrix - depends on $x_1, \ldots, x_n$ but not $y_1, \ldots, y_n$.

- Then the **effective number of parameters** is defined as

$$\boxed{\text{df}(\mathbf{S}) = \text{trace}(\mathbf{S})}$$

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2. $\hat{y} = (\hat{y}_1, \ldots, \hat{y}_n)$ is the vector of predictions,
3. $\mathbf{S}$ is an $n \times n$ matrix - depends on $x_1, \ldots, x_n$ but not $y_1, \ldots, y_n$.

- Then the **effective number of parameters** is defined as

$$\boxed{\text{df}(\mathbf{S}) = \text{trace}(\mathbf{S})}$$

General definition: Effective degrees-of-freedom

- If y arises from an additive-error model

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

  with $\mathsf{Var}(\epsilon) = \sigma_\epsilon^2$ then

$$\sum_{i=1}^{n} \mathsf{Cov}(\hat{y}_i, y_i) = \mathsf{trace}(\mathbf{S})\sigma_\epsilon^2$$

- The more general definition of **effective dof** is then

$$\boxed{\mathsf{df}(\hat{y}) = \frac{\sum_{i=1}^{n} \mathsf{Cov}(\hat{y}_i, y_i)}{\sigma_\epsilon^2}}$$

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The Bayesian Approach and BIC

Generic form of BIC

Bayesian Information Criterion

$$\boxed{\text{BIC} = -2\,\text{loglik} + \log(n)\,d}$$

- Assuming **Gaussian model** and known variance σ_ϵ^2 then

$$-2\,\text{loglik} = \frac{1}{\sigma_\epsilon^2}\sum_{i=1}^{n}(y_i - \hat{h}(x_i))^2 = \frac{n\,\overline{\text{err}}}{\sigma_\epsilon^2}$$

  and

$$\boxed{\text{BIC} = \frac{n}{\sigma_\epsilon^2}\left(\overline{\text{err}} + \log(n)\,\frac{d}{n}\sigma_\epsilon^2\right)}$$

- Note BIC $\propto$ AIC, but BIC penalizes complex model more heavily than AIC.

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Derivation of BIC

- **Starting point:**

  Have $\{\mathcal{M}_1, \dots, \mathcal{M}_M\}$ a set of candidate models and their corresponding parameters $\theta_1, \dots, \theta_m$.

- **Goal:**

  Choose the best model $\mathcal{M}_i$.

- **How:**

  - Have training data $\mathbf{Z} = \{(x_1, y_1), \dots, (x_n, y_n)\}$
  - Have priors $p(\theta_m|\mathcal{M}_m)$.
  - The posterior of model $\mathcal{M}_m$ is

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\begin{aligned}
P(\mathcal{M}_m|\mathbf{Z}) &\propto P(\mathcal{M}_m)\, p(\mathbf{Z}|\mathcal{M}_m) \\
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- Usually assume uniform prior: $P(\mathcal{M}_m) = 1/M$.
- Approximate the above integral by simplification and Laplace approximation to get

$$\log P(\mathbf{Z}|\mathcal{M}_m) = \log P(\mathbf{Z}|\hat{\theta}_m, \mathcal{M}_m) - \frac{d_m}{2} \log n + O(1)$$

  where $\hat{\theta}_m$ is a MLE and d_m is # free parameters in $\mathcal{M}_m$.
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AIC Vs BIC

- If $\mathcal{M}_{\text{true}} \in \{\mathcal{M}_1, \ldots, \mathcal{M}_M\}$ then as $n \to \infty$
  - BIC will select $\mathcal{M}_{\text{true}}$. ✓
  - AIC will not. It tends to choose too complex models as $n \to \infty$. ✗
- However, when n is small
  - BIC often chooses models which are too simple. ✗

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Cross-Validation

K-Fold Cross-Validation

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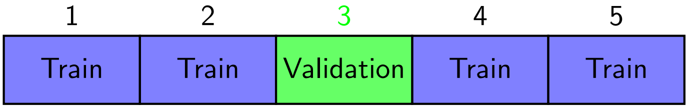
General Approach

- Split the data into K roughly equal-size parts.



- For the kth part calculate the prediction error of the model fit using the other $K-1$ parts.

- Do this for $k = 1, 2, \ldots, K$ and combine the K estimates of the prediction error.

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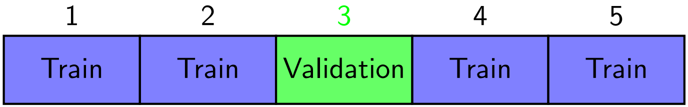

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When and why

- It is applied when labelled training data is relatively sparse.

- This method directly estimates $\text{Err} = \mathsf{E}[L(Y, \hat{f}(X))]$.

K-Fold Cross-validation: Detailed description

- The mapping $\kappa : \{1, \ldots, n\} \to \{1, \ldots, K\}$ indicates observation i belongs to partition $\kappa(i)$.

- $\hat{f}^{-k}(x)$ is the function fitted with the kth part of the data removed.

- **Cross-validation** estimate of the prediction error is

$$\boxed{\mathrm{CV}(\hat{f}) = \frac{1}{n} \sum_{i=1}^{n} L(y_i, \hat{f}^{-\kappa(i)}(x_i))}$$

- Typical choices for K are 5 or 10.

- The case $K = n$ is known as leave-one-out cross-validation.

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K-Fold Cross-validation: Model selection

- Have models $f(x, \alpha)$ indexed by a parameter α.
- $\hat{f}^{-k}(x, \alpha)$ is αth model fit with kth part of the data removed.
- Then define

$$\boxed{\mathrm{CV}(\hat{f}, \alpha) = \frac{1}{n} \sum_{i=1}^{n} L(y_i, \hat{f}^{-\kappa(i)}(x_i, \alpha))}$$

- Choose the model

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What quantity does K-fold validation estimate?

Intuition says

- When $K = 5$ or 10 then $CV(\hat{f}) \approx \mathrm{Err}$ as training sets for each fold are fairly different.

- When $K = n$ then $CV(\hat{f}) \approx \mathrm{Err}_{\mathcal{T}}$ as training sets for each fold are almost identical.

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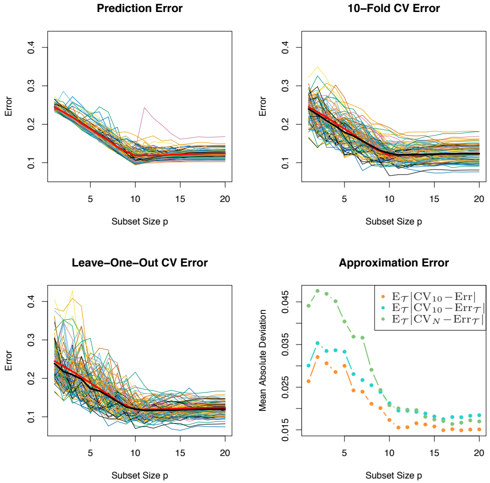
Book's simulation experiments say

- Cross-validation, really only effectively estimates Err.

What quantity does K-fold validation estimate?



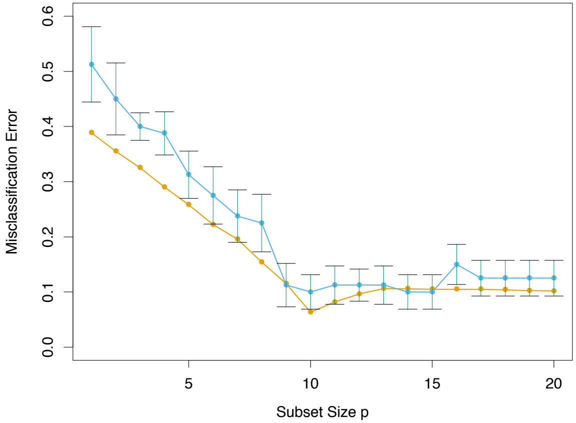
- **Thick red curve: $\mathbf{Err}$**
- **Thick black curve: $\mathrm{E}_{\mathcal{T}}[\mathrm{CV}_K]$**

What value of K?

- When $K = n$
  - $CV(\hat{f})$ is approx an unbiased estimate of Err. ✓
  - $CV(\hat{f})$ has high variance as the n *training sets* are similar. ✗
  - Computational burden is high. ✗ (except for a few exceptions)
- When $K = 5$ (is lowish)
  - $CV(\hat{f})$ has low variance. ✓
  - $CV(\hat{f})$ is potentially an upward biased estimate of Err. ✗

    Only occurs if at each fold there is not enough training data to fit a good model.

Example of a K-fold cross validation curve



- Orange curve: $\mathrm{Err}_{\mathcal{T}}$
- Blue curve: $\mathrm{CV}_{10}(\hat{f})$

Right & Wrong way to do Cross-validation

Classification problem with a large # of predictors

What's wrong with this strategy?

1. Screen the predictors Find a subset of *good* predictors that are correlated with the class labels.
2. Build a classifier based on the subset of good predictors.
3. Perform cross-validation to estimate the unknown tuning parameters and to estimate Err of the final model.

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The good predictors were chosen after seeing all the data.

Should have done this

1. Divide the samples into K groups randomly.

2. For each fold $k = 1, \ldots, K$

    - Find a subset of *good* predictors using all the samples minus the kth fold.

    - Build a classifier using all the samples minus the kth fold.

    - Use the classifier to predict the labels for the samples in the kth fold.

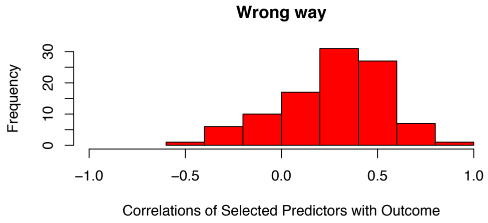
Example

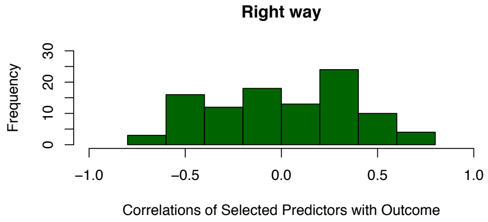
Set-up

- Have a binary classification problem.
- $n = 50$ with an equal number of points from each class.
- Have $p = 5000$ quantitative predictors that are independent of the class labels.
- The true error rate of any classifier is 50%.

✗ If one performs pre-selection of 100 predictors and then builds a 1-nn classifier the average CV error rate was 3% over 50 simulations ! ✗

Example: correlation of class labels with predictors





To perform Multistep Modelling

- Cross-validation must be applied to the entire sequence of modelling steps.
- Samples must be **left out** before any selection or filtering is applied which uses the labels.
- One exception: An unsupervised screening step can use all the samples.

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Bootstrap Method

- Have a training set $\mathbf{Z} = (z_1, z_2, \ldots, z_n)$ with each $z_i = (x_i, y_i)$.
- The **bootstrap** idea is

```
for $b = 1, 2, \ldots, B$
    1. Randomly draw $n$ samples with replacement from $\mathbf{Z}$ to get $\mathbf{Z}^{*b}$ that is
           $\mathbf{Z}^{*b} = (z_{b_1}, z_{b_2}, \ldots, z_{b_n})$   with $b_i \in \{1, \ldots, n\}$
    2. Refit the model using $\mathbf{Z}^{*b}$ to get $S(\mathbf{Z}^{*b})$
Examine the behaviour of the $B$ fits
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Can estimate any aspect of the distribution of $S(\mathbf{Z})$

- For example its variance

$$\boxed{\widehat{\mathrm{Var}}[S(\mathbf{Z})] = \frac{1}{B-1}\sum_{b=1}^{B}(S(Z^{*b}) - \bar{S}^{*})^2}$$

where

$$\bar{S}^{*} = \frac{1}{B}\sum_{b=1}^{B} S(Z^{*b})$$

Use Bootstrap to estimate Prediction Error

Attempt 1

$$\boxed{\widehat{\text{Err}}_{\text{boot}} = \frac{1}{B}\frac{1}{n}\sum_{b=1}^{B}\sum_{i=1}^{n} L(y_i, \hat{f}^{*b}(x_i))}$$

where $\hat{f}^{*b}(x_i)$ is the predicted value at x_i using the model computed from $\mathbf{Z}^{*b}$.

- Why is this not a good estimate??
  - Overlap between training and test sets
- How could we do better?
  - Mimic cross-validation

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Attempt 2: Leave-one-out bootstrap

$$\boxed{\widehat{\text{Err}}^{(1)} = \frac{1}{n}\sum_{i=1}^{n}\frac{1}{|C^{-i}|}\sum_{b\in C^{-i}} L(y_i, \hat{f}^{*b}(x_i))}$$

where C^{-i} is the set of bootstrap samples b not containing observation i.

- Either make
- Make B large enough so $|C^{-i}| > 0$ for all i **or**
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Is the leave-one-out prediction any good?

- **Pros**:
  1. avoids the overfitting problem of $\widehat{\text{Err}}_{\text{boot}}$
- **Cons**:
  1. Has the training-set-size bias of cross-validation
  2. The $P(\text{observation } i \in \mathbf{Z}^{*b})$ is
     $$1 - \left(1 - \frac{1}{n}\right)^n \approx 1 - e^{-1} = .632$$
     Therefore the average number of distinct observations in $\mathbf{Z}^{*b}$ is $.632\, n$.
  3. $\widehat{\text{Err}}^{(1)}$'s bias is thus similar to twofold cross-validation.

To alleviate this bias

Attempt 3: The .632 estimator

$$\boxed{\widehat{\text{Err}}^{(.632)} = .368\,\overline{\mathsf{err}} + .632\,\widehat{\text{Err}}^{(1)}}$$

- Compromise between the **training error** $\overline{\mathsf{err}}$ and the **leave-one-out bootstrap** estimate.
- Its derivation is not easy.
- Obviously the constant .632 relates to $P(\text{observation } i \in \mathbf{Z}^{*b})$.

The .632 estimator **does not do well** if predictor **overfits**.

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Estimate the degree of overfitting

No-information error rate:

$$\boxed{\hat{\gamma} = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} L(y_i, \hat{f}(x_j))}$$

- Estimate of the error rate of $\hat{f}$ if inputs and outputs were independent.
- Note the prediction rule, $\hat{f}$, is evaluated on all possible combinations of targets y_i and predictors x_j.

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Estimate the degree of overfitting

Relative overfitting rate:

$$\boxed{\hat{R} = \frac{\widehat{\mathrm{Err}}^{(1)} - \overline{\mathsf{err}}}{\hat{\gamma} - \overline{\mathsf{err}}}}$$

- $0 \leq \hat{R} \leq 1$
- $\hat{R} = 0 \implies$ no overfitting.
- $\hat{R} = 1 \implies$ overfitting equals no-information value $\hat{\gamma} - \overline{\mathsf{err}}$.

Use Bootstrap to estimate Prediction Error

Attempt 4: The .632+ estimator

$$\boxed{\widehat{\text{Err}}^{(.632+)} = (1 - \hat{w})\,\overline{\text{err}} + \hat{w}\,\widehat{\text{Err}}^{(1)}}$$

with

$$\hat{w} = \frac{.632}{1 - .368\hat{R}}$$

- $.632 \le \hat{w} \le 1$ as $\hat{R}$ ranges from 0 to 1.
- $\widehat{\text{Err}}^{(.632+)}$ ranges from $\widehat{\text{Err}}^{(.632)}$ to $\widehat{\text{Err}}^{(1)}$.
- $\widehat{\text{Err}}^{(.632+)}$ is a compromise between $\widehat{\text{Err}}^{(.632)}$ and $\overline{\text{err}}$ that depends on the amount of overfitting.
- Derivation of the above eqn is non-trivial.

Use Bootstrap to estimate Prediction Error

Attempt 4: The .632+ estimator

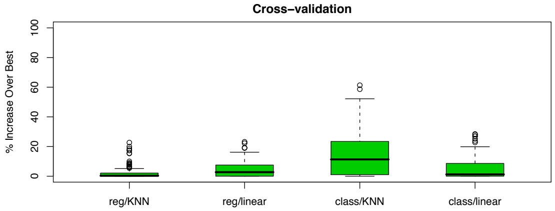
$$\boxed{\widehat{\text{Err}}^{(.632+)} = (1-\hat{w})\,\overline{\text{err}} + \hat{w}\,\widehat{\text{Err}}^{(1)}}$$

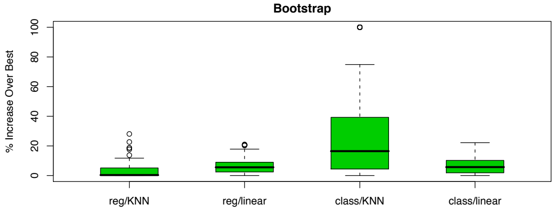
with

$$\hat{w} = \frac{.632}{1 - .368\hat{R}}$$

- $.632 \le \hat{w} \le 1$ as $\hat{R}$ ranges from 0 to 1.
- $\widehat{\text{Err}}^{(.632+)}$ ranges from $\widehat{\text{Err}}^{(.632)}$ to $\widehat{\text{Err}}^{(1)}$.
- $\widehat{\text{Err}}^{(.632+)}$ is a compromise between $\widehat{\text{Err}}^{(.632)}$ and $\overline{\text{err}}$ that depends on the amount of overfitting.
- Derivation of the above eqn is non-trivial.

How bootstrap and cv perform wrt model selection





- Boxplots show $100\frac{\mathrm{Err}(\hat{\alpha}) - \min_{\alpha}\ \mathrm{Err}(\alpha)}{\max_{\alpha}\ \mathrm{Err}(\alpha) - \min_{\alpha}\ \mathrm{Err}(\alpha)}$ where $\hat{\alpha}$ is the best parameter found via the selection method under investigation.
- 100 training sets were used.