Statistical Machine Learning
Part 6

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Resampling Methods for Parameter Estimation

Suppose you have applied your state of the art algorithm, but you don't know what is the distribution of a parameter (hyperparameter). The question is: how do I determine the bias and variance?
The **jackknife** and **bootstrap** are *resampling* methodologies that help improving classification.

Jacknife

It was introducied by Maurice Quenouille around 1950's. Let's start with an example as motivation for the use of the jacknife.
Example. Let's suppose that we have m independent random variables $X_1, \ldots, X_m$ that follow the same distribution. We can define the statistic $\overline{X}$ defined as $\frac{X_1+\cdots+X_m}{m}$. The question is what is the standard deviation of this statistic given a set of observed values $X_1 = x_1, \ldots, X_m = x_m$?
Following the definition of variance, we can determine

$$\widehat{\sigma}^2(\overline{X}) = \frac{1}{m(m-1)} \sum_{i=1}^{m} (x_i - \overline{x})^2 \tag{1}$$

That was simple enough, but what about calculating an estimate of the variance for other common statistics as *mode*, or *median* or other statistics?

Jackknife

Let's define the sample average of the data set deleting the jth variable as

$$\overline{X}_{(j)} = \frac{1}{m-1} \sum_{k \neq j} X_k$$

We also define the statistic that is the *average* of these averages

$$\overline{X}_{(\bullet)} = \frac{1}{m} \sum_{k=1}^{m} \overline{X}_{(k)}$$

The **Jackknife** estimate of the standard deviation is

$$\widehat{\sigma}^2_{Jack}(\overline{X}) = \frac{m-1}{m} \sum_{i=1}^{m} (\overline{X}_{(i)} - \overline{X}_{(\bullet)})^2 \qquad (2)$$

It can be verified that (1) and (2) coincide; however, this process allows a generalization of this method.

Jackknife

One of the biggest advantages of the expression (2) is that when we have an estimator $\hat{\theta}(x_1, \ldots, x_m)$ of the statistic θ, we can actually estimate the variance of such estimator

$$\hat{\sigma}^2_{jack} = \frac{m-1}{m} \sum_{i=1}^{m} (\hat{\theta}_{(i)} - \hat{\theta}_{(\bullet)})^2,$$

where

$$\hat{\theta}_{(i)} = \hat{\theta}(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_m)$$

$$\hat{\theta}_{(\bullet)} = \frac{1}{m-1} \sum_{i=1}^{n} \hat{\theta}_{(i)}$$

Jackknife bias

It is also possible to obtain the **jackknife bias** estimation
Recall the definition of bias

$$bias = \theta - E(\hat{\theta})$$

The Jackknife estimate of bias is given by

$$bias_{jack} = (m-1)(\hat{\theta}_{(\bullet)} - \hat{\theta})$$

Bootstrap

In a common definition, a *bootstrap* data set is one created by randomly selecting m points (with replacement) from the training set $\mathcal{D}$.
For example if our training data set consists of the points $\{(x_1, y_1), (x_2, y_2), (x_3, y_3)\}$, then a bootstrap could be

$$B_1 = \{(x_1, y_1), (x_2, y_2), (x_3, y_3)\}$$
$$B_2 = \{(x_1, y_1), (x_1, y_1), (x_2, y_2)\}$$
$$B_3 = \{(x_2, y_2), (x_3, y_3), (x_2, y_2)\}$$

Bootstrap

The bootstrap was developed by Bradley Efron in the late 1970s. In the bootstrap setup, the data sets (say B_js in our example) are treated as independent sets. The **bootstrap** estimate of a statistic θ is defined as

$$\hat{\theta}^{*(\bullet)} = \frac{1}{B} \sum_{b=1}^{B} \hat{\theta}^{*(b)},$$

where $\hat{\theta}^{*(b)}$ is the estimate of θ for the sample b .

Bootstrap bias and variance estimates

The bootstrap estimate of the bias

$$bias_{boot} = \hat{\theta}^{*(\bullet)} - \hat{\theta}$$

Whereas the bootstrap estimate of the variance is

$$\hat{\sigma}^2(\theta) = \frac{1}{B} \sum_{b=1}^{B} \left(\hat{\theta}^{*(b)} - \hat{\theta}^{*(\bullet)} \right)$$

Subset Selection (Regression)

We have seen than when several predictors are present, it is difficult to determine which ones to keep or discard.
There are some alternatives:

- Best Subset Selection
- Stepwise Selection
  - Forward Selection
  - Backwards Selection

Best Subset Selection (Regression)

Let's suppose we have a linear regression model

$$Y = \theta_0 + \theta_1 X_1 + \cdots + \theta_p X_p + \varepsilon$$

In theory, we can make (loads) of models

$$\begin{aligned}
\mathcal{M}_0 &: \hat{Y} = \hat{\theta}_0 \\
\mathcal{M}_1 &: \hat{Y} = \hat{\theta}_0 + \hat{\theta}_1 X_1 \\
&\vdots \\
\mathcal{M}_p &: \hat{Y} = \hat{\theta}_0 + \hat{\theta}_1 X_1 \\
\mathcal{M}_{p+1} &: \hat{Y} = \hat{\theta} + \hat{\theta}_1 X_1 + \hat{\theta}_2 X_2 \\
&\vdots \\
\mathcal{M}_{2^p-1} &: \hat{Y} = \hat{\theta}_0 + \hat{\theta}_1 X_1 + \cdots + \hat{\theta}_p X_p
\end{aligned}$$

Best Subset Selection

Algorithm for Best Subset Selection

1. For $k \in \{1, \ldots, p\}$:
   - 1.1 Fit all $\binom{p}{k}$ models that contain exactly k predictors.
   - 1.2 Pick the best among these $\binom{p}{k}$ models, and call it $\widehat{\mathcal{M}}_k$. The selection is based either by selecting the smallest RSS, or largest R^2.
2. Select a single best model from among $\mathcal{M}_0, \widehat{\mathcal{M}}_1, \ldots, \widehat{\mathcal{M}}_p$ using cross-validated prediction error, C_p (AIC), BIC, or adjusted R^2.

Notice that in step 3 we have changed our metric. If we were to proceed with the same metric (say largest R^2), we will end up with the model including all parameters since R^2 increases monotonically towards 1 as the number of predictors increases.

Forward Stepwise Selection

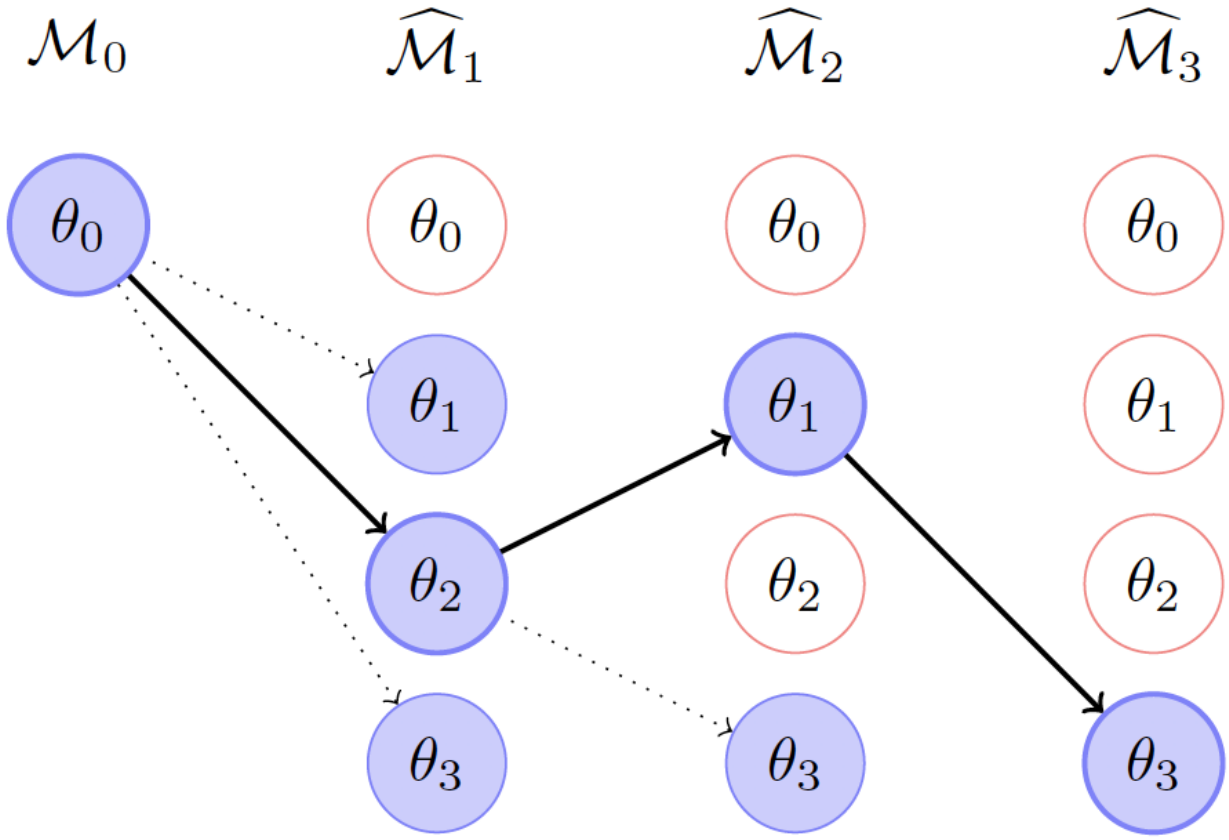
The algorithm for this problem is stated as

1. For $k = \{0, \ldots, p-1\}$:
   - 1.1 Consider all $p-k$ models that augment the predictors in $\widehat{\mathcal{M}}_k$ with one additional predictor.
   - 1.2 Choose the *best* among these $p-k$ models and call it $\widehat{\mathcal{M}}_{k+1}$. The metric is defined as having the smallest RSS or highest R^2.
2. Select a single best model from among $\mathcal{M}_0, \widehat{\mathcal{M}}_1, \ldots, \widehat{\mathcal{M}}_p$ using corss-validated prediction error C_p (AIC), BIC, or adjusted R^2.

So, instead of comparing 2^p models, we will be comparing $1 + \frac{p(p+1)}{2}$ models.

Note that the forward stepwise tends to do well in practice, it is not guaranteed to find the best possible model!

Forward Stepwise Selection

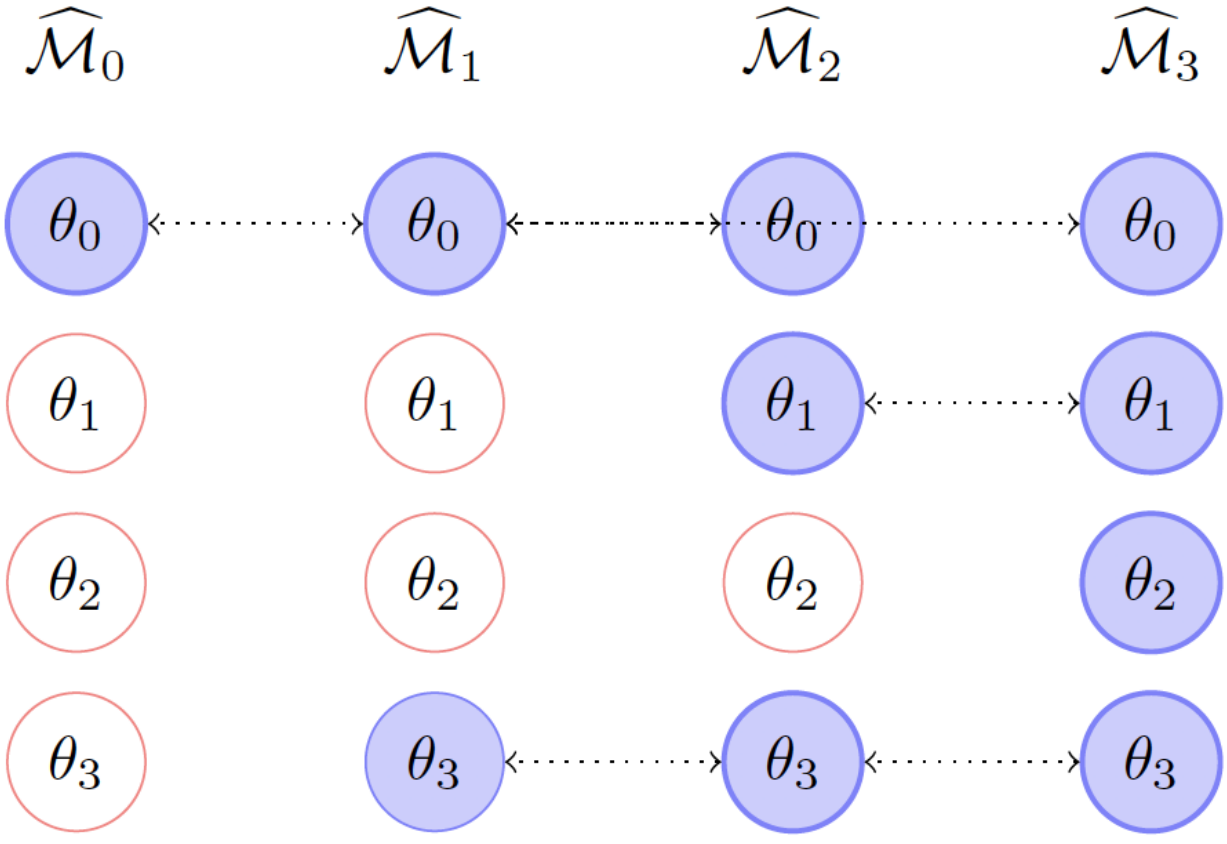


Backwards Stepwise Selection

It requires the same number of steps as the forward selection. The algorithm runs as follows:

1. Let $\widehat{\mathcal{M}}_p$ denote the full model with all predictors.
2. For $k = p, p-1, \ldots, 1$:
   - Consideer all k models that contain all but one of the predictors in $\widehat{\mathcal{M}}_k$, for a total of $k-1$ predictors.
   - Choose the *best* among these k models, and call it $\widehat{\mathcal{M}}_{k-1}$. Again, we consider one of the metrics such as the smallest RSS or largest R^2.
3. Select a single best model from among $\mathcal{M}_0, \widehat{\mathcal{M}}_1, \ldots, \widehat{\mathcal{M}}_p$ using cross-validated prediction error, C_p (AIC), BIC or adjusted R^2.

Backwards Stepwise Selection



Selection criteria

Let's suppose we have fitted a model containing d predictor, the C_p estimate of test MSE is computed using the equation

$$C_p = \frac{1}{n}(RSS + 2d\hat{\sigma}^2),$$

where $\hat{\sigma}^2$ is an estimate of the variance of the error ε associated with each response measurement. C_p is an unbiased estimate of test MSE. Thus, we choose the model with the lowest C_p value. The Akaike information criteria (AIC) is defined for a large class of models fit by maximum likelihood.

$$AIC \approx \frac{1}{n\hat{\sigma}^2}(RSS + 2d\hat{\sigma}^2)$$

The Bayesian information criteria (BIC) is derived from a Bayesian point of view

$$BIC \approx \frac{1}{n}(RSS + \log(n)d\hat{\sigma}^2)$$

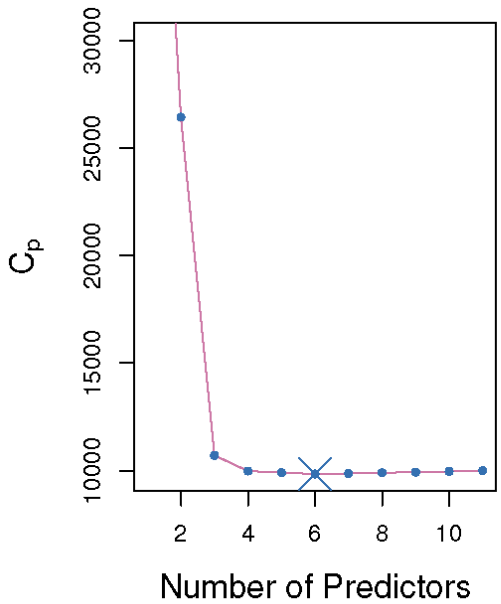
Adjusted R^2

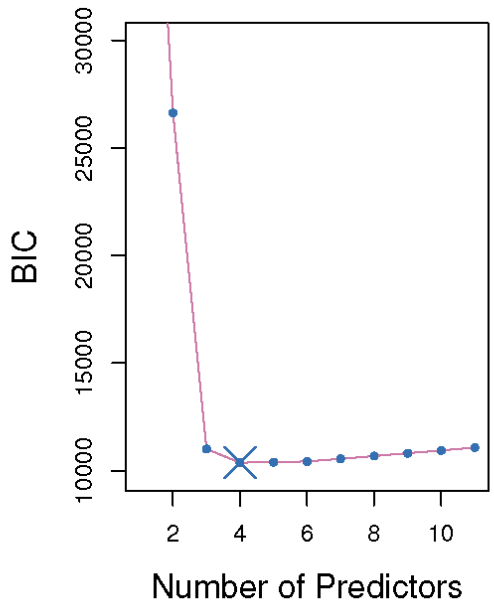
Finally, the so-called **adjusted** R^2 statistic is defined as

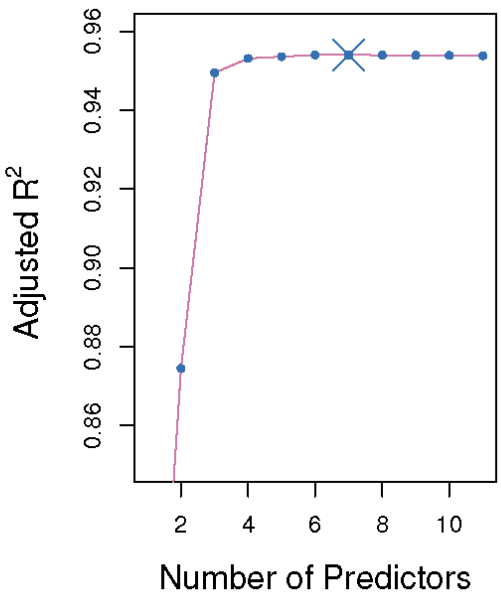
$$\text{Adjusted } R^2 = 1 - \frac{RSS/(n-d-1)}{TSS/(n-1)} = 1 - \frac{n-1}{n-d-1} \cdot \frac{RSS}{TSS}$$

Recall that $R^2 = 1 - RSS/TSS$ where $TSS = \sum(y_i - \bar{y})^2$ is the total sum of squares. So adding the adjusted R^2 statistic pays a price for the inclusion of unnecessary variables in the model.

Optimal Selection







Final Thoughts

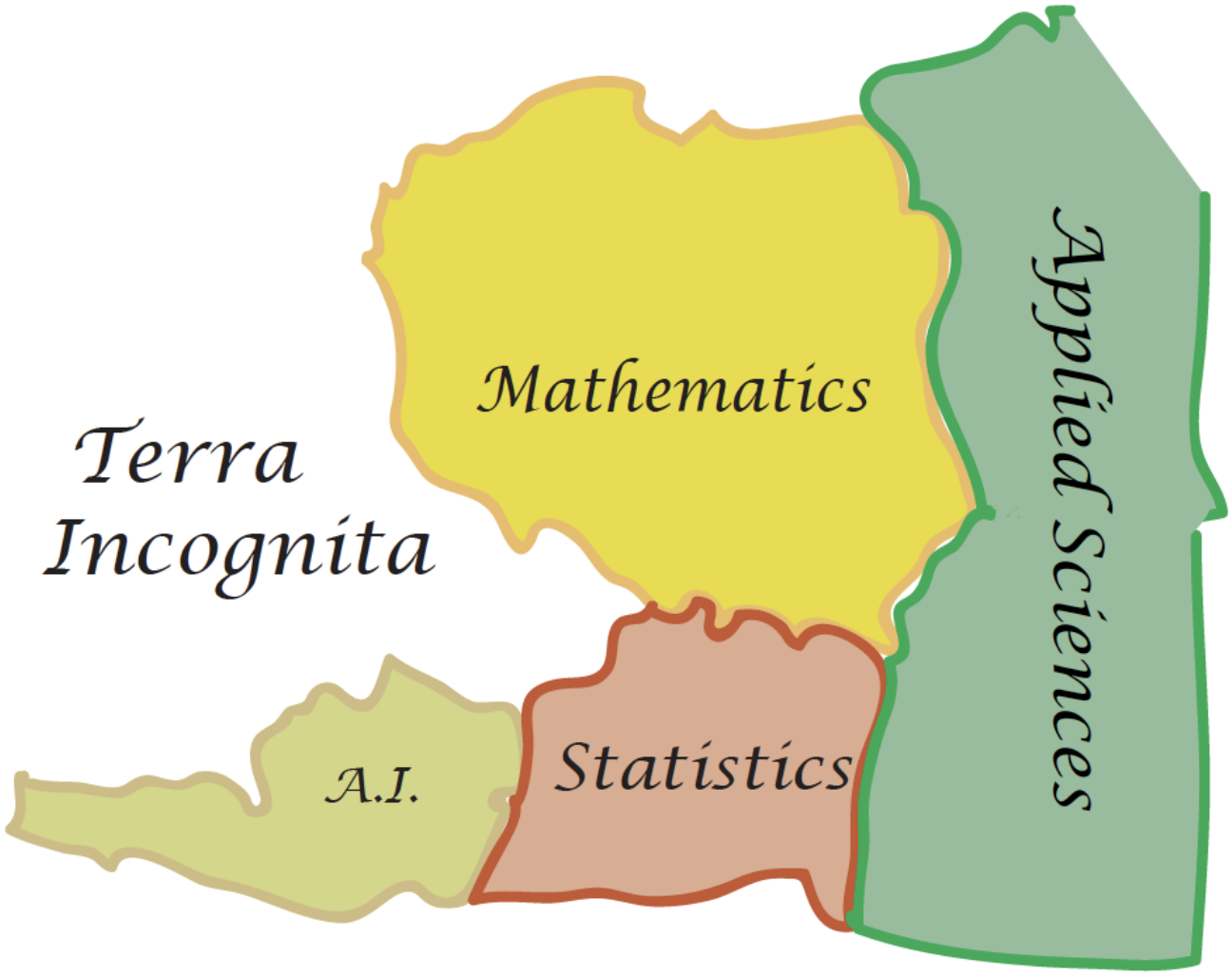


FIGURE 1. The greater world of mathematics and science.

References

Materials and some of the pictures are from (1),(2), and (3).

1. Gareth James et al. *An Introduction to Statistical Learning with applications in R*. Springer (2015)
2. Richard O. Duda et al. *Pattern Classification* John Wiley (2001).
3. Aurélien Géron. *Hands-on Machine Learning with Scikit-Learn & TensorFlow* O'Relly (2017)
4. Wiebe R. Pestman *Mathematical Statistics* de Gruyter (1998)
5. Bradley Efron. *The Jackknife, the Bootstrap and other Resampling Plans* SIAM (1982)
6. Bradley Efron *A 250-year argument: Belief, behavior and the bootstrap* Bull. Am. Math. Soc (2012)

I have used some of the graphs by hacking TiKz code from StakExchange, Inkscape for more aesthetic plots and other old tricks of TEX