Resampling methods for error rate estimation in supervised learning

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Outline

1. Error rate estimation
2. Resubstitution error rate
3. Holdout approach
4. Cross-validation
5. Bootstrap
6. Influence of the sampling scheme

Measuring the performance of the classifiers

The inability to measure the true error rate on the whole population

Starting point: We have a sample of size "n" as from which we want to build a classifier M(n)

$$\hat{Y} = M(X, n)$$

Prediction error rate: The "true" error rate can be obtained by the comparison of the observed values of Y and the prediction of the classifier M on the whole population.

$$\varepsilon = \frac{\sum_{\omega \in \Omega_{pop}} [Y(\omega) \neq \hat{Y}(\omega)]}{card(\Omega_{pop})}$$

Error rate computed on the entire population = probability of misclassification of the classifier

But: (1) The "whole" population is never available

(2) Accessing to all the instances is too costly

How to do by having in everything and for everything the sample of size "n" to learn the model and to measure its performance ...

Measuring the performance of the classifiers

Illustration with the "waves" dataset – Breiman and al. (1984)

Description:

- One target variable (3 classes of waves) and 21 continuous predictive attributes
- Generated dataset - Potentially of infinite size
- n = 500 instances, used for the learning process
- n = 500,000 instances, the “population” used for measuring the “true” error rate (baseline measure)
- 3 learning algorithms (LDA, C4.5 and Perceptron) which have various behaviors

The “true” error rate: measured on the “population” (500,000 instances)

	Erreur "théorique" (Calculé sur 500000 obs.)
LDA	0.185
C4.5	0.280
RNA (10 CC)	0.172

In practice, we have never an unlimited number of instances. Thus, we must use the available sample (n = 500) instances in order to learn the model and estimate its error rate. For each classifier, the estimated error rate must be as close as possible to the "true" value above.

Resubstitution error rate

Use the same dataset for the learning phase and the evaluation phase

Steps:

- Learn the classifier on the sample (n= 500)
- Apply the classifier on the same sample
- Build the confusion matrix and calculate the error rate

→ This is the resubstitution error rate.

$$e_r = \frac{\sum_{\omega \in \Omega} [Y(\omega) \neq \hat{Y}(\omega)]}{n}$$

Results

	Erreur "théorique"	Erreur Resubstitu
LDA	0.185	0.124
C4.5	0.280	0.084
RNA (10 CC)	0.172	0.064

Comments:

- The resubstitution error rate underestimates very often the true error rate
- The gap depends on the characteristics of the dataset AND classifier
- More a point influences its own affectation, more the optimism bias will be high

→ (1) NN, 1-NN : resubstitution error rate = 0% is possible, etc.

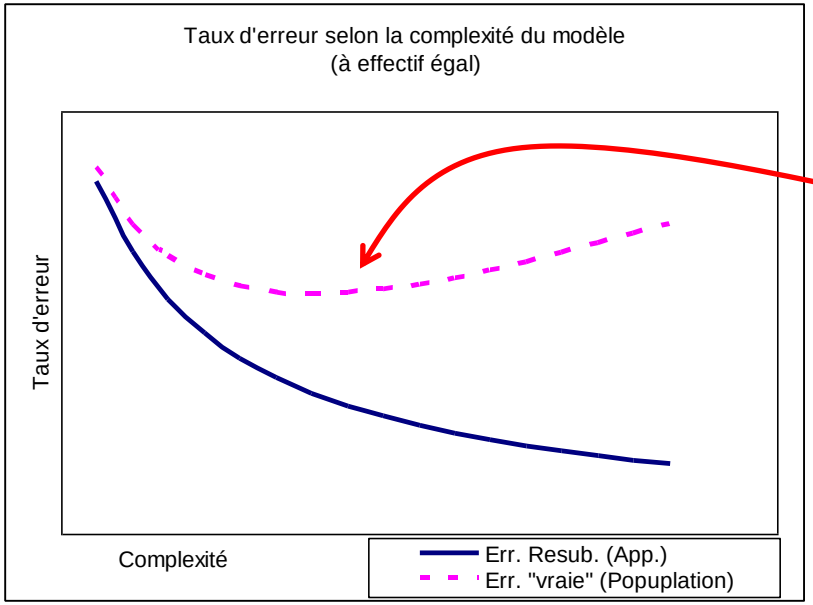
→ (2) Classifiers with high complexity

→ (3) Small sample size (n is low)

→ (4) High dimensionality (in relation to the sample size) and noisy variables

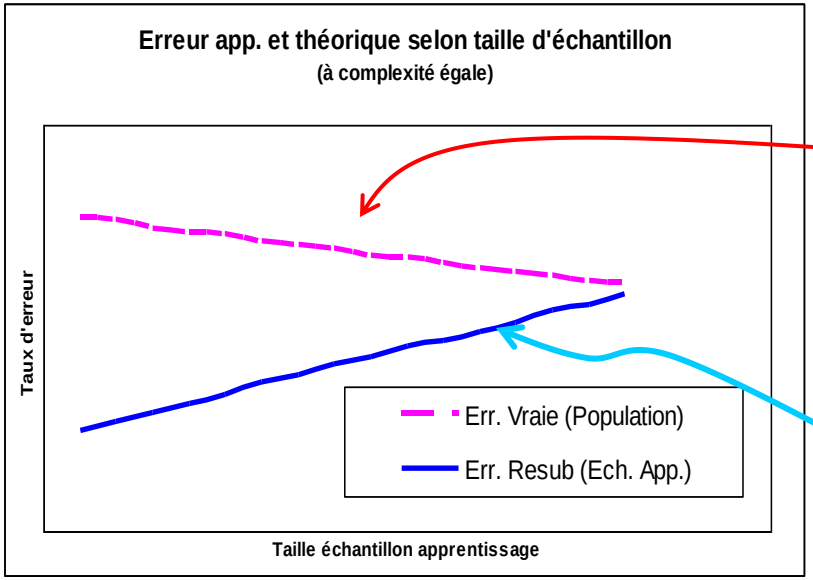
Behavior of the resubstitution error rate (blue) and the true error rate (purple)

According to the complexity of the classifier and the sample size



The algorithm begins to learn sample-specific "patterns" that are not true to the population

(e.g. too many variables. too many neurons in the hidden layer; too large decision tree...)



The larger is the sample size, the more efficiently we learn the "underlying relationship" between X and Y in the population

The larger is the sample size, the less is the dependence of the algorithm to the sample singularities.

The holdout approach

Split the dataset into train sample and test sample

Learning phase, train set

Ω_a

$n_a \approx 60\% \sim 70\%$

$M(X, n_a)$

Ω

n

Dataset

Ω_t

$n_t \approx 30\% \sim 40\%$

Testing phase, test set

$$e_t = \frac{\sum_{\omega \in \Omega_t} [Y(\omega) \neq \hat{Y}(\omega)]}{n_t}$$

Test error rate

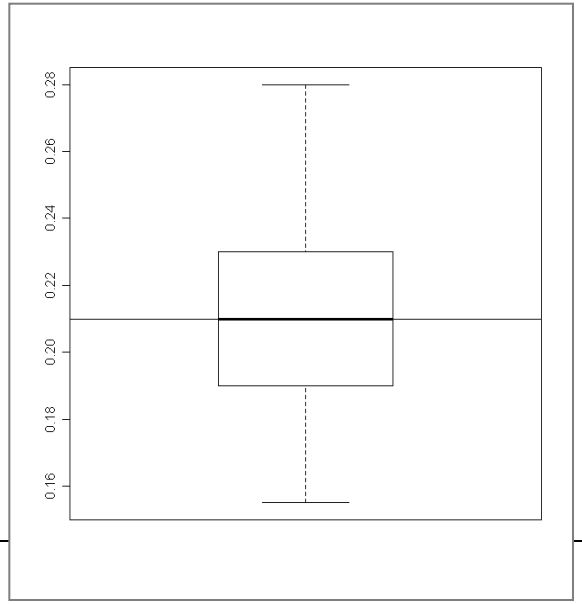
Unbiased estimation of the $M(X,n_a)$ error rate

Modèle : LDA(X,300) → $\varepsilon = 0.2099$ Computed on the 500,000 instances

Test set : 200 obs. → $\varepsilon = 0.1950$

Experiments

Repeat 100 times the process
300 inst. train, 200 inst. test →



The holdout approach

Bias and variance

e_t is an **unbiased** estimation of the error rate of $M(X, n_a)$ LDA(X,300)

But This is a **biased** estimation of the error of $M(X, n)$ LDA(X,500)

Large train set and large test set are not compatible.

Part of the data only (300 inst.) is used to learn the model, the learning is of lower quality than if we use the whole sample with n = 500 inst.

The "bias" is lower when the train sample is larger.

Bias

The test error rate is accurate when the test sample size is high. The larger is the test sample, the lower is the variance.

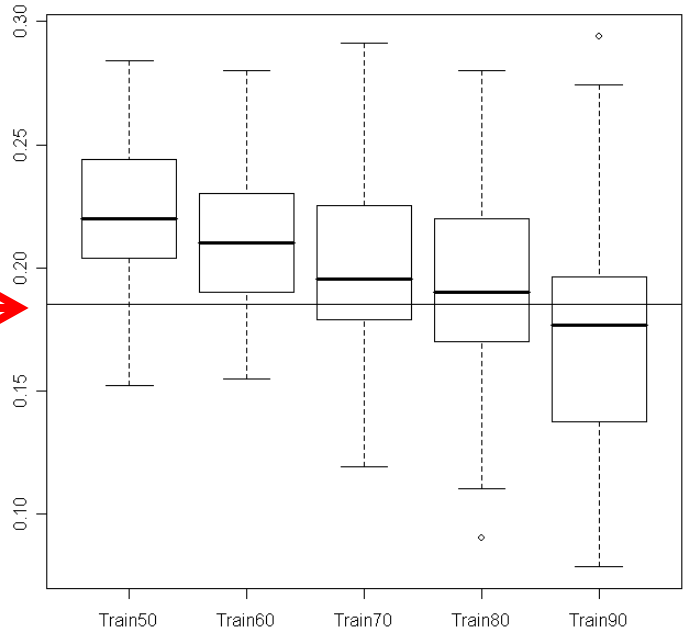
Variance

The holdout approach

Experiments

The train sample size increases

"True" error rate of
LDA(X,500) = 0.185



High bias
Low variance

Low bias
High variance

Conclusion:

- The test error rate is an unbiased estimation of the performance of the classifier learned on the train sample.
- But it is a bad estimation of the performance of the classifier learned on the whole dataset
- The holdout approach is only interesting when we handle large database
- Otherwise, we are facing a dilemma: increase the train sample size to obtain a good model but bad error evaluation, or increase the test sample size to obtain a better error rate estimation of a bad model.

How to estimate the error of M(X,n) ?

Resampling techniques

Cross-validation
Leave-one-out
Bootstrap

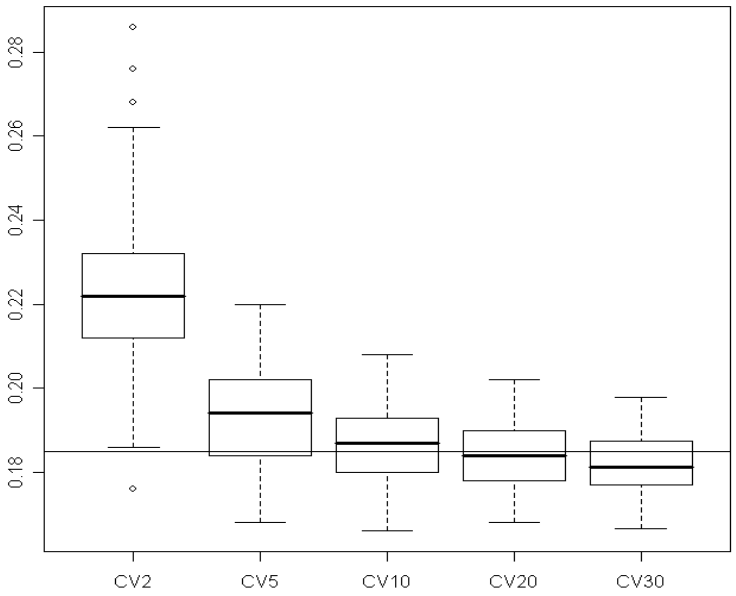
Cross-validation

Principle

Algorithm

- Subdivide the sample in K folds (groups) – n_k is the size of the k^{th} fold
- For each k :
  - Construct the model M(X,n-n_k)
  - Calculate its test error rate on n_k → e_k
- e_{cv} = the mean of the errors e_k

"True" error rate of LDA(X,500) = 0.185



- K=10 gives a good compromise between "bias" and "variance" for the most of the situations (dataset and learning algorithm)

- Repeated cross-validation may improve its characteristics (B x K-Fold Cross validation)

- In the case of overfitting, the cross-validation (especially when K is high) tends to underestimate the true error rate

Leave-one-out

Special case of cross-validation where K = n

Algorithm

- Subdivide the sample into K=n folds
- For each instance k :
  - Construct the classifier M(X,n-1)
  - Apply the classifier on the k^{th} instance → e_k
- Calculate the mean e_{loo} of the errors

e_k = 1 (error) or 0 (good prediction)

Proportion of errors

- Significantly more computationally expensive than the K (K << n) cross validation without being best
- Dramatically underestimate the error rate in the case of overfitting

Experiments (with the sample of size 500)

	Erreur "théorique" (Calculé sur 500000 obs.)	10-CV	Leave one out
LDA	0.185	0.170	0.174
C4.5	0.280	0.298	0.264
RNA (10 CC)	0.172	0.174	0.198

We can decrease the variance by repeating the process

Only one measurement is possible on a sample of size n.

Algorithm

- Repeat B times (called “replications”)
  - Sample with replacement a dataset of size n → Ω_b
  - Separate the unselected instances → $\Omega_{(b)}$
  - Construct the classifier with the dataset Ω_b
  - Calculate the resubstitution error rate on Ω_b [$e_r(b)$]
  - Calculate the test error rate on $\Omega_{(b)}$ [$e_t(b)$]
  - Calculate the “optimism” o_b

On the whole dataset (size n), calculate the resubstitution error rate

(1) $$e_B = e_r + \frac{\sum_b o_b}{B}$$

$\mathbf{e_r}$ is the resubstitution error rate
The bootstrap enables to estimate the "optimism"
It is used to correct the resubstitution error rate
The correction is often a little excessive
(the error is often overestimated with the standard bootstrap)

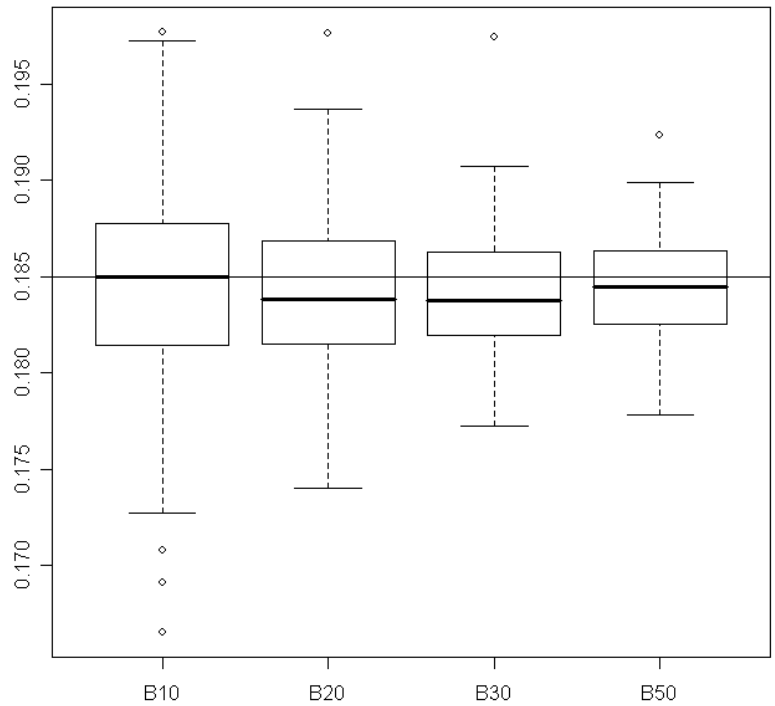
(2) $$e_{0.632B} = 0.368 \times e_r + 0.632 \times \frac{\sum_b e_t(b)}{B}$$

0.632 bootstrap
→Weight with the probability of belonging to Ω_b for a replication (#0.632)
The correction is more realistic

(3) It exists another approach which allows to correct the "optimism" by taking account the classifier characteristic: 0.632+ bootstrap

Experiments -- 0.632 Bootstrap

Increase the number of replication



"True" error rate
LDA = 0.185

Decreasing of the variance – B # 25 is enough
Little influence on the bias

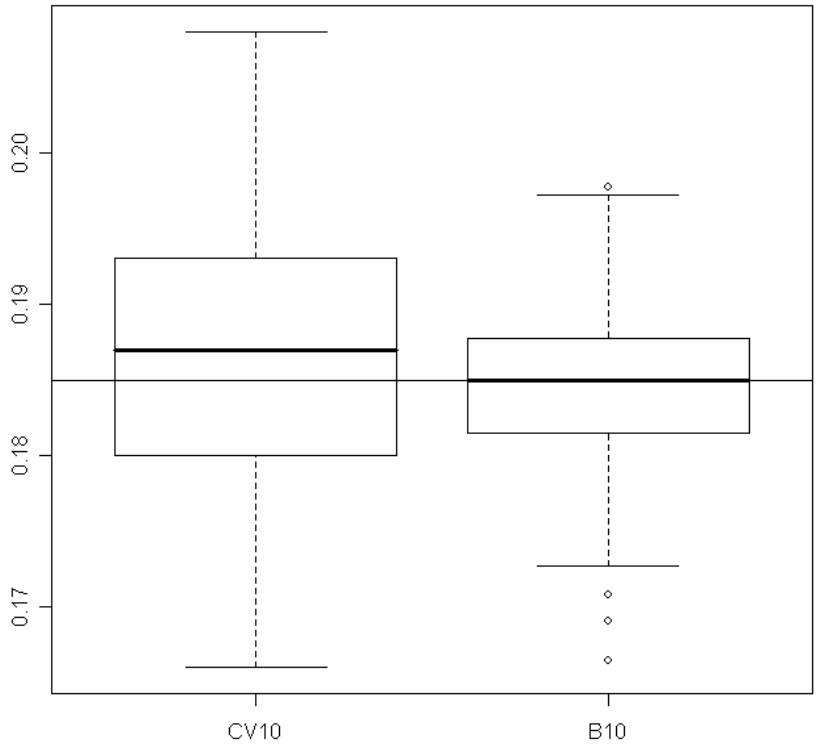
The bias comes from the fact that, with each replication, n instances well used to construct the model, but as some instances are repeated, the information is redundant, the model is less efficient... we cannot modify this behavior ...

Cross-validation or bootstrap ?

At equal cost calculation (here 10 repetitions of the train-test operations)

- Bootstrap has lower variance

- But the cross-validation is less biased (we have a counter-example here, but it is only a simulation with 100 repetitions on one dataset and one kind of classifier)



In scientific publications, researchers seem to favor cross-validation ... maybe because it is easier to implement.

Sampling scheme

Influence of the sampling method on the organization of the cross-validation

Stratified sampling, cluster sampling, etc.

General principle: the mode of constitution of the folds must respect the sampling method for the constitution of the dataset

→ If the dataset comes from a stratified sampling from the population, we must use the same way for the selection of instances in each fold e.g. defining the same proportion of the classes in each fold

Goal: decrease the variance

→ If the dataset comes from a cluster sampling, the sample unit becomes the clusters in order to constitute the folds

Goal: decrease the bias

Conclusion

- Resubstitution error is (almost) always too optimistic i.e. underestimates the true error rate
- This optimism depends on the characteristics of the data and the classifier

- The holdout approach is only interesting on large dataset (number of instances)
- The test error estimates the performance of the classifier learned on the train sample
- But it gives a bad indication about the performance of the classifier learned from the whole dataset

- Cross-validation and bootstrap are equivalent in general
- K = 10 seems a good compromise for the cross-validation
- Repeated cross-validation decreases the variance, but not in a spectacular way

- 0.632 bootstrap has a lower variance than the cross-validation, but higher bias
- We cannot really correct this bias (the 0.632+ can handle this but it is not very common in software)

- In the case of overfitting, both cross-validation and bootstrap cannot give a good estimation of the error rate

References

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A. Molinaro, R. Simon, R. Pfeiffer, « Prediction error estimation: a comparison of resampling methods », in Bioinformatics, 21(15), pages 3301-3307, 2005 http://bioinformatics.oxfordjournals.org/cgi/content/full/21/15/3301