Machine Learning

Module 5: Data Splitting

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Overfitting

A good model should have the good metric (predictions) and a good capacity to extrapolate outside the data base.

Consider the following stupid but feasible model to predict an instance:

- if the instance is already in the data base, the predicted class is the same as the one in the data base.
- if the instance is not already in the data base, the prediction is random.

The model will have a perfect accuracy on the data base. However, it is useless for new instances.

Overfitting

This example illustrates that it is easy to build good predictions when the data base is available: predicting the past is easy.

In the context of a supervised learning, a model may be good at predicting the data base on which it is trained but not the future/other data points. In practice however, this **generalization capacity** is crucial.

A model having very good predictions on the data base, and a poor extrapolation capacity (for new instances) is said to **overfit** the data.

Overfitting is one of the worst enemy in machine learning: it looks like things are going well, when in fact no good new predictions can be obtained.

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Concept

The simplest data split consists of:

1. A **training set** on which the models are trained;
2. A **test set** on which predictions are tested.

Concept

Often,

- The split is **random** (assignment of the instances).
- The two sets are **disjoint**: no common instance, except if they are already multiple in the data base.
- Common proportions Tr/Te are like 75/25 or 80/20.
- However, with very large data base, it is useless to have too large training set. With millions of data points, often a 10% training set is enough (if the data are representative and rich enough).

Apparent and test metrics

- On the training set, the metrics (accuracies, etc.) are called **apparent metrics**: often too optimistic.
- The test set they are called **test metrics**: close to the one expected when the model will be in use on new data.

To **detect** overfitting, for a positive metric (e.g., accuracy),

- If $Metric(Tr) >> Metric(Te)$: overfitting.
- If $Metric(Tr) \approx Metric(Te)$: no sign of overfitting.

Exceptionally, "apparent underfitting" is possible: $Metric(Tr) < Metric(Te)$. This is unlikely. It can be due to chance (e.g., with small data set) or sometimes information leakage (e.g., selection of hyperparameters based on the test set).

Example

A data set with 1000 instances,

- Split at random:
  - training set of 750 instances,
  - Test set of 250 instances.
- A logistic regression is fitted to the training set.
- The features of the test set are given to the model to make the test set predictions. These are compared to the correct classes in the test set.
- The apparent (left) and test (right) confusion matrices:

```
          Reference
Prediction Bad Good
      Bad   30   19
      Good 195  506
```

```
          Reference
Prediction Bad Good
      Bad    6    7
      Good  69  168
```

Example

The apparent and test accuracies are

$$A_{tr} = \frac{30 + 506}{750} = 0.715, \quad A_{te} = \frac{6 + 168}{250} = 0.696.$$

The accuracy on the test set is closer to the one that can be expected if the model was used on new instances.

Here, the test accuracy is lower than the apparent accuracy. This is a usual sign of over-fitting[1].

[1] Mild though.

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Validation set

When the training set is split further into a training set[2] and a **validation set**.

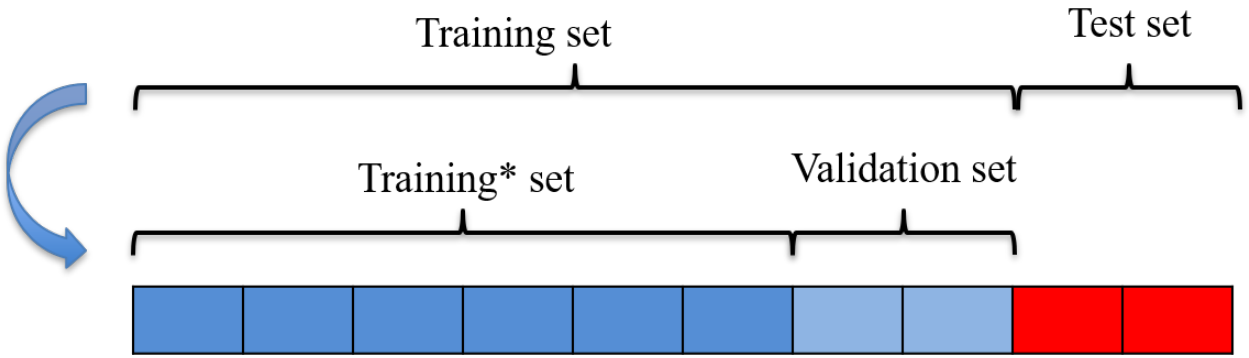
- Several models are trained on this smaller training set
- The best model is selected based on the metrics obtained on the validation set.
- The test metric of best model is computed to have a final evaluation of what this metric will be on new data.

This avoids **information leakage**: using the best model on the test set can cause overfitting of this test set...

Validation set is also used for cross-validation, hyperparameter selection, early stopping, etc. See below.

[2] There is no specific name to distinguish between the first "big" training set, and the second one, that is smaller.

Illustration



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Repeated splits

One single training/validation/test split taken at random can be unstable or impossible to replicate: the randomness was badly balanced or too much dependence on this specific split.

Repeated splits can be used to address this issue. They are under two forms:

- **Cross-validation** (CV).
- **Bootstrap**.

K-fold CV

1. Split the data set into non-overlapping K subsets,
2. For each $k = 1, \ldots, K$,
   - Use subset k as the validation set, and the rest of the data set as the training set,
   - Train the model on the training set
   - Compute the predictions on the validation set
   - Compute and record the metric S_k

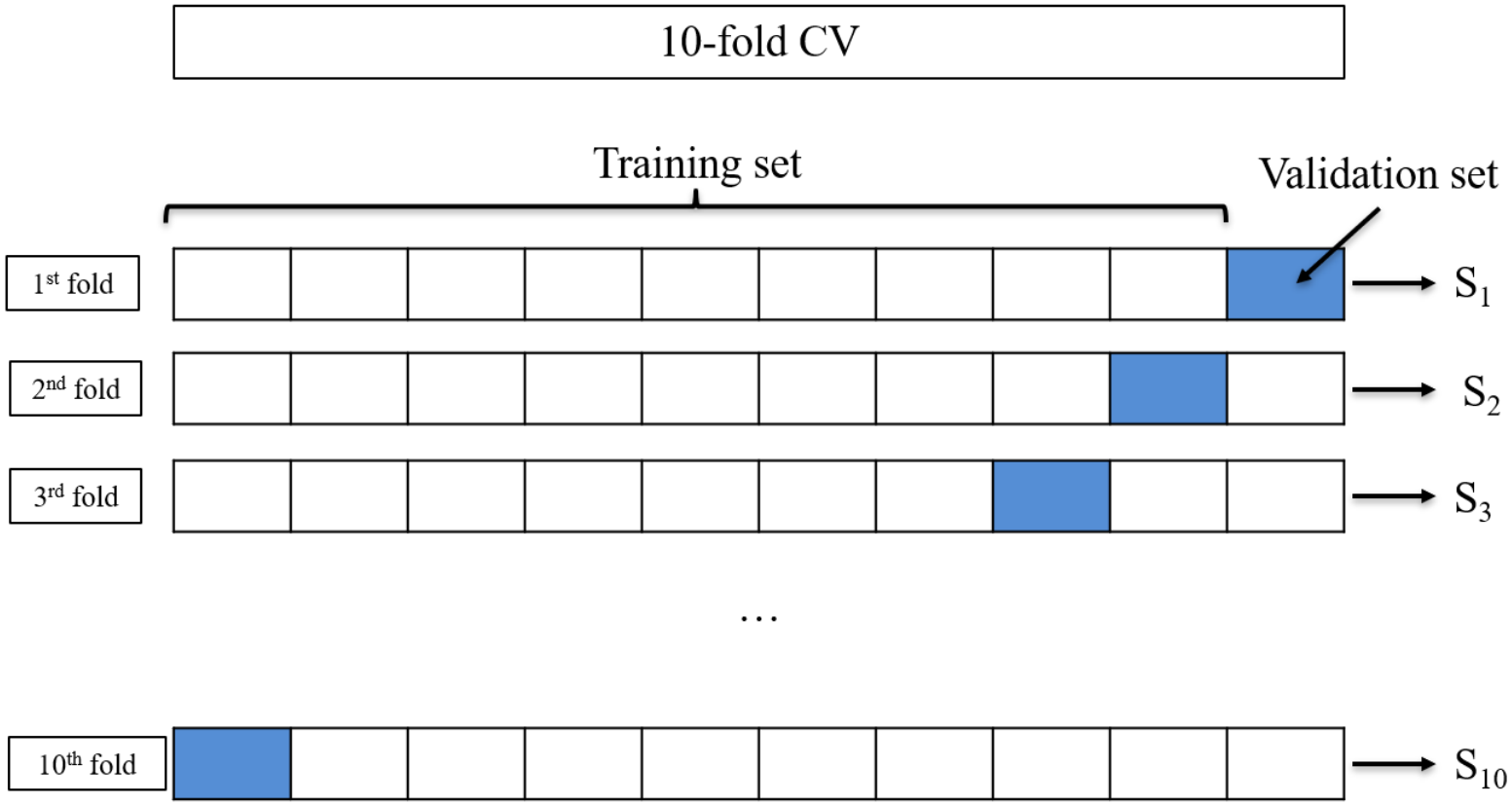
This provides K metrics: $S_1, \ldots, S_K$. The final CV metric is their average:

$$\hat{S} = \frac{1}{K} \sum_{k=1}^{K} S_k.$$

In addition, these metrics are used to estimate the standard deviation[3] of $\hat{S}$.

[3] Technically, this is the method used in 1-SE rule for trees.

K-fold CV



Reproduced from https://sebastianraschka.com/faq/docs/evaluate-a-model.html

Example

A 10-fold CV is made. The accuracies of are logistic regression in each fold are

S_1	S_2	S_3	S_4	S_5	S_6	S_7	S_8	S_9	S_{10}
0.63	0.71	0.73	0.73	0.76	0.64	0.71	0.75	0.78	0.69

The CV accuracy (standard deviation) is 0.713 (0.049).

On the same data split, another model gives CV accuracy of 0.654 (0.053).

The logistic regression should be preferred here.

K-fold CV

How to choose K?

- No universal good choice. In practice, use $K = 5$ or $K = 10$.
- A special case is $K = n$, known as **leave-one-out** (LOO).
- If a more specific choice of K is needed, then look for a trade-off between
  - computational capacity: large K gives more iterations and larger training sets, thus longer computation.
  - number of validation metrics: large K gives more S_k so $\hat{S}$ is well estimated.
  - number of data to train the model: large K gives large training set thus better estimated models.
  - number of data to estimate the validation metric: large K gives small validation set, thus S_k is not well estimated.

Bootstrap: Re-sampling

In context of ML, **bootstrap** stands for **re-sampling with replacement**. It is an alternative to CV. The differences between CV and bootstrap are

- for CV, the whole data base is split once. Training and validation sets do not have common instances.
- For bootstrap, the training and validation sets vary in size and composition at each step.

The fact that instances can be repeated in the training set can create a bias. A weighted estimate tackles this issue: the **632-rule**.

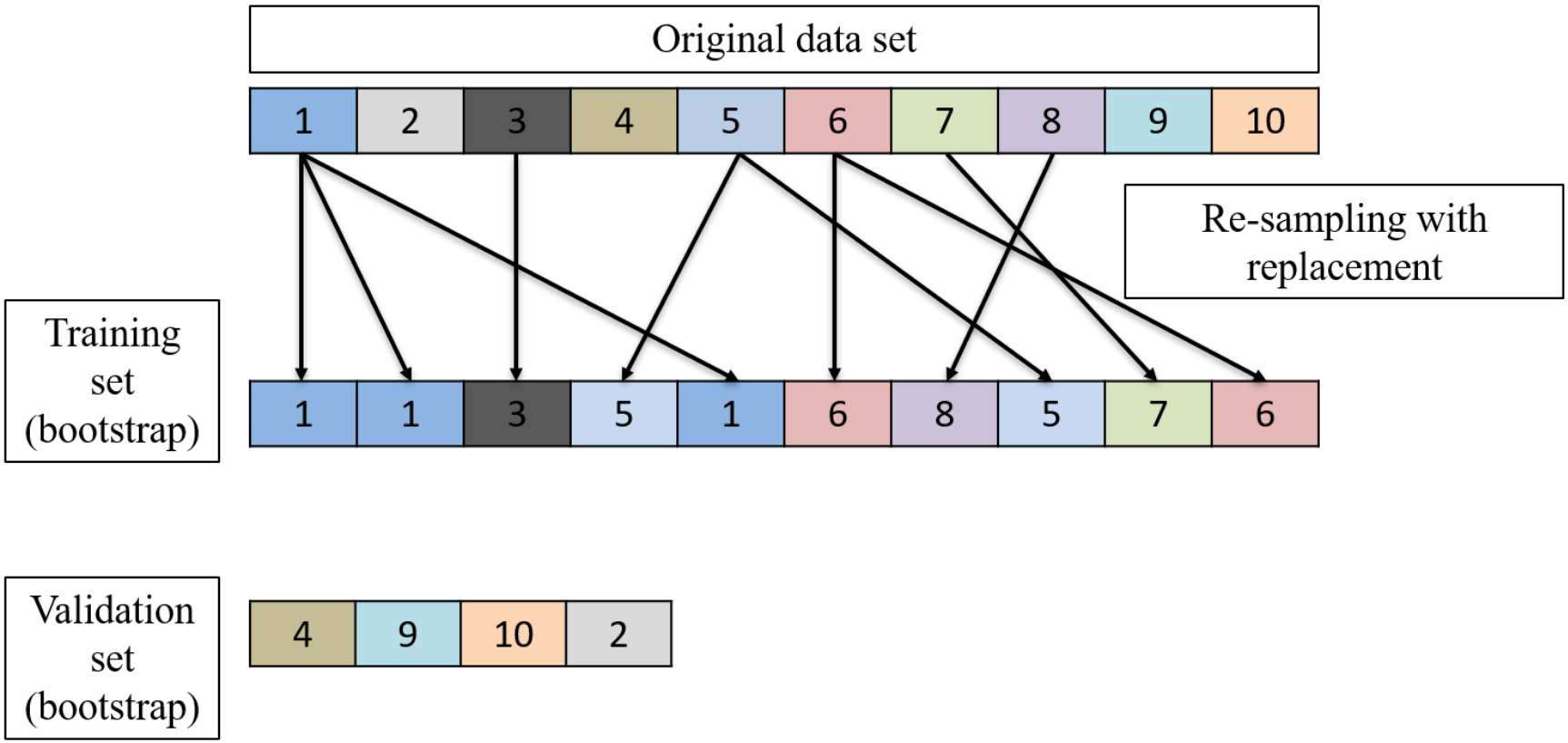
Bootstrap: Procedure

In practice, one bootstrap step consists of

1. Select at random a training set by sampling from the original data base, *with replacements*, and *of the same size*.
2. The instances in the original data base *that are not in the generated training set* constitute the validation set.
3. Compute the metric on the validation set after having trained the model with the training set: **out-of-bag** metric, $\hat{S}_{oob}$.
4. Compute also the prediction of the training set itself: **apparent** metric, $\hat{S}_{app}$.
5. Estimate the metric using the **632-rule**:

$$\hat{S} = 0.632 \times \hat{S}_{oob} + 0.368 \times \hat{S}_{app}.$$

One bootstrap step



Bootstrap estimate

The previous bootstrap step is repeated a large number of times; typically 500 to 10'000, depending on the time it takes (computation power).

The final estimate is the average of each $\hat{S}$. Standard deviation can be also computed.

Bootstrap samples

How many bootstrap samples (R) should be used?

- There is no theoretical number but people consider that it should be at least large enough so that all the instances of the data base are at least once selected in a validation set.
- In practice, a large number depending on the computational power and the size of the data set.

Practical use

In practice,

- With small data base, prefer bootstrap over CV.
- With large data base, prefer CV over bootstrap
- CV can be repeated: several CV pattern are simulated independently and aggregated at the end.
- These procedures can be computed in parallel for better performance.
- CV is more commonly used.

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Solving overfitting

Comparing apparent and test metrics allows only to detect overfitting. How can we improve the situation?

Models overfitting the training data set are too flexible or complex. We can use the methods seen for each model to try to simplify them:

- Linear and logistic regression: variable selection and/or use L_1 and L_2 penalization.
- Trees: prune the tree.
- SVM: tune the cost parameter and/or the parameters of the kernel.
- NN: use L_1 and L_2 penalization, simplify the structure of the network, use early stopping.

Hyperparameters

Some of these methods require to set parameters: penalization parameter, cost parameter, others.

These are called **hyperparameters**. Hyperparameters are structural parameters or "pseudo-parameters" of the models.

An informal definition is "whatever cannot be optimized by the training algorithm".

Setting these parameters is called **tuning**.

Tuning hyperparameters

The main technique consists of direct comparison (brute force):

- Create a list of possible hyperparameter values.
- Train all the models from the list.
- Select the best in class according to the validation metric.

This approach can be done on

- A simple split: training set and validation set.
- A repeated split: bootstrap or CV.

The choice of the hyperparameters must not be done on the test set: a part of the information contained in the test set may *leaks* to the model choice and thus to the training.

$\Rightarrow$ To avoid any **information leakage**: the **test set must not be seen** by the model, at any stage.

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Unbalanced classes

"Unbalanced classes" refers to data set where the classes frequencies are unbalanced. E.g., doctor visit data have 4 times more "No" than "Yes".

```
  No  Yes
4141 1049
```

During the training, the model favors the predictions of the "No" to reach a better accuracy.

Unbalanced classes

E.g., the logistic regression, gives:

```
Confusion Matrix and Statistics
[...]
               Accuracy : 0.8091
[...]
            Sensitivity : 0.9771
            Specificity : 0.1435
[...]
      Balanced Accuracy : 0.5603
```

This problem is **detected** with

- low balanced accuracy
- low sensitivity or specificity

Tuning probability threshold

One approach to solve this issue is to tune the probability threshold λ:

$$f(x_i;\theta) = \begin{cases} 1, & \text{if } p(x_i;\theta) > \lambda, \\ 0, & \text{if } p(x_i;\theta) \leq \lambda. \end{cases}$$

To maximize the balanced accuracy, find the threshold λ that maximizes the **Youden's J statistics**:

$$J(\lambda) = \text{Spec}(\lambda) + \text{Sens}(\lambda) - 1.$$

Note: this optimization is always at the cost of a lower accuracy.

Tuning probability threshold

Example after optimization:

```
Confusion Matrix and Statistics
[...]
               Accuracy : 0.6991
[...]
            Sensitivity : 0.7186
            Specificity : 0.6220
[...]
      Balanced Accuracy : 0.6703
```

Sensitivity decreased, specificity increased. Overall BA increased (and accuracy decreased).

The probability threshold λ is an hyperparameter. Use the splitting data method to avoid overfitting or information leakage.

Class balancing

Another approach consists of **balancing** the classes *in the training set*. Two possible approaches:

- **Sub-sampling**: Remove cases in the training set,
- **Re-sampling**: Add cases in the training set.

Class balancing

In details

- Sub-sampling: take all the "Yes" and a random subset of "No" of the same size.
- Re-sampling: take all the "No" and add replicates of the "Yes", chosen at random, until there are as many "Yes" as "No".

Variations are possible to increase or decrease the weight of each class, to take into account for the proportions.

Note: **Never balance the test set**.

Class balancing

Example,

With sub-sampling

```
               Accuracy : 0.7049
[...]
            Sensitivity : 0.7331
            Specificity : 0.5933
[...]
      Balanced Accuracy : 0.6632
```

With re-sampling

```
               Accuracy : 0.7097
[...]
            Sensitivity : 0.7391
            Specificity : 0.5933
[...]
      Balanced Accuracy : 0.6662
```

The results are similar to tuning of λ.

Discussion on class balancing

- Case imbalance is a common problem in real life data (fraud detection, rare events, etc.).
- Applied on the data, class balancing is a possible solution to improve the fit.
- Unlike tuning of the probability threshold, class balancing can be apply to no-probability models and multi-class problems.
- There is no guarantee. The final performances must be inspected.
- **The test set must remain unbalanced** to be representative of future data.
- If you use CV or bootstrap, the validation set must remain unbalanced (often not the case in built-in methods).