Training, test, and validation sets

In machine learning, the study and construction of algorithms that can learn from and make predictions on data[1] is a common task. Such algorithms work by making data-driven predictions or decisions,[2]:2 through building a mathematical model from input data.

The data used to build the final model usually comes from multiple datasets. In particular, three data sets are commonly used in different stages of the creation of the model.

The model is initially fit on a **training dataset**,[3] that is a set of examples used to fit the parameters (e.g. weights of connections between neurons in artificial neural networks) of the model.[4] The model (e.g. a neural net or a naive Bayes classifier) is trained on the training dataset using a supervised learning method (e.g. gradient descent or stochastic gradient descent). In practice, the training dataset often consist of pairs of an input vector and the corresponding *answer* vector or scalar, which is commonly denoted as the *target*. The current model is run with the training dataset and produces a result, which is then compared with the *target*, for each input vector in the training dataset. Based on the result of the comparison and the specific learning algorithm being used, the parameters of the model are adjusted. The model fitting can include both variable selection and parameter estimation.

Successively, the fitted model is used to predict the responses for the observations in a second dataset called the **validation dataset**.[3] The validation dataset provides an unbiased evaluation of a model fit on the training dataset while tuning the model's hyperparameters [5] (e.g. the number of hidden units in a neural network[4]). Validation datasets can be used for regularization by early stopping: stop training when the error on the validation dataset increases, as this is a sign of overfitting to the training dataset.[6] This simple procedure is complicated in practice by the

fact that the validation dataset's error may fluctuate during training, producing multiple local minima. This complication has led to the creation of many ad-hoc rules for deciding when overfitting has truly begun.[6]

Finally, the **test dataset** is a dataset used to provide an unbiased evaluation of a *final* model fit on the training dataset.[5]

Confusingly the terms **test dataset** and **validation dataset** are sometimes used with swapped meaning. As a result it has become commonplace to refer to the set used in iterative training as the **test/validation set** and the set that is used for hyperparameter tuning as the **holdout set**.

Training dataset

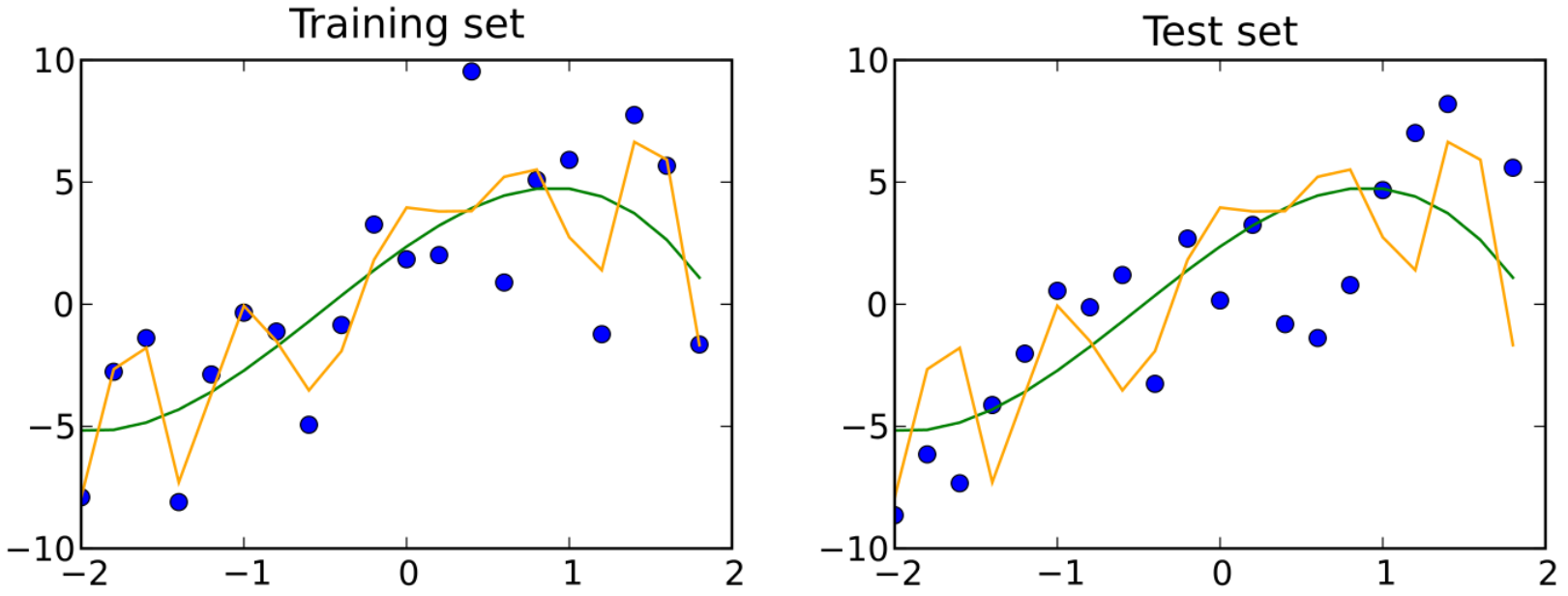
A training dataset is a dataset of examples used for learning, that is to fit the parameters (e.g., weights) of, for example, a classifier.[7][8]

Most approaches that search through training data for empirical relationships tend to overfit the data, meaning that they can identify apparent relationships in the training data that do not hold in general.

Test dataset

A test dataset is a dataset that is independent of the training dataset, but that follows the same probability distribution as the training dataset. If a model fit to the training dataset also fits the test dataset well, minimal overfitting has taken place (see figure below). A better fitting of the training dataset as opposed to the test dataset usually points to overfitting.

A test set is therefore a set of examples used only to assess the performance (i.e. generalization) of a fully specified classifier.[7][8]



A training set (left) and a test set (right) from the same statistical population are shown as blue points. Two predictive models are fit to the training data. Both fitted models are plotted with both the training and test sets. In the training set, the MSE of the fit shown in orange is 4 whereas the MSE for the fit shown in green is 9. In the test set, the MSE for the fit shown in orange is 15 and the MSE for the fit shown in green is 13. The orange curve severely overfits the training data, since its MSE increases by almost a factor of four when comparing the test set to the training set. The green curve overfits the training data much less, as its MSE increases by less than a factor of 2.

Validation dataset

A validation dataset is a set of examples used to tune the hyperparameters (i.e. the architecture) of a classifier. It is sometimes also called the development set or the "dev set". In artificial neural networks, a hyperparameter is, for example, the number of hidden units.[7][8] It, as well as the testing set (as mentioned above), should follow the same probability distribution as the training dataset.

In order to avoid overfitting, when any classification parameter needs to be adjusted, it is necessary to have a validation dataset in addition to the training and test datasets. For example, if the most suitable classifier for the problem is sought, the training dataset is used to train the candidate algorithms, the validation dataset is used to compare their performances and decide which one to take and, finally, the test dataset is used to obtain[*citation needed*] the performance characteristics such as accuracy, sensitivity, specificity, F-measure, and so on. The validation dataset functions as a hybrid: it is training data used by testing, but neither as part of the low-level training nor as part of the final testing[*citation needed*].

The basic process of using a validation dataset for model selection (as part of training dataset, validation dataset, and test dataset) is:[8][9]

> Since our goal is to find the network having the best performance on new data, the simplest approach to the comparison of different networks is to evaluate the error function using data which is independent of that used for training. Various networks are trained by minimization of an appropriate error function defined with respect to a training data set. The performance of the networks is then compared by evaluating the error function using an independent validation set, and the network having the smallest error with respect to the validation set is selected. This approach is called the *hold out* method. Since this procedure can itself lead to some overfitting to the validation set, the performance of the selected network should be confirmed by measuring its performance on a third independent set of data called a test set.

An application of this process is in early stopping, where the candidate models are successive iterations of the same network, and training stops when the error on the validation set grows, choosing the previous model (the one with minimum error).

Holdout dataset

In practice the terms "test set" and "validation set" are used interchangeably (flipped from how they are described above). As a result it's become common to refer to the one that is used during training to be referred to as *either* the test/validation set. To disambiguate, the set that gets set aside for hyperparameter tuning (here described as the *validation set*) is generally referred to as the **holdout set**.

Selection of a holdout dataset

Holdout method

Most simply, part of the training dataset can be set aside and used as a validation set: this is known as the **holdout method**[10].

Cross-validation

Alternatively, the *hold out* process can be repeated, repeatedly partitioning the original training dataset into a training dataset and a validation dataset: this is known as cross-validation. These repeated partitions can be done in various ways, such as dividing into 2 equal datasets and using them as training/validation, and then validation/training, or repeatedly selecting a random subset as a validation dataset[*citation needed*].

Cross-validation doesn't work in situations where you can't shuffle your data. For example, for an image classifier, if you have a series images in the dataset that are similar and you put half in test and half in training, you will end up inflating the performance metrics of your classifier.

Hierarchical classification

Another example of parameter adjustment is **hierarchical classification** (sometimes referred to as **instance space decomposition** [11]), which splits a complete multi-class problem into a set of smaller classification problems. It serves for learning more accurate concepts due to simpler classification boundaries in subtasks and individual feature selection procedures for subtasks. When doing classification decomposition, the central choice is the order of combination of smaller classification steps, called the classification path. Depending on the application, it can be derived from the confusion matrix and, uncovering the reasons for typical errors and finding ways to prevent the system make those in the future. For example,[12] on the validation set one can see which classes are most frequently mutually confused by the system and then the instance space decomposition is done as follows: firstly, the classification is done among well recognizable classes, and the difficult to separate classes are treated as a single joint class, and finally, as a second classification step the joint class is classified into the two initially mutually confused classes.

See also

- Cross-validation (statistics)
- Machine learning
- Statistical classification
- List of datasets for machine learning research

References

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External links

- FAQ: What are the population, sample, training set, design set, validation set, and test set?
- What is the Difference Between Test and Validation Datasets?
- What is training, validation, and testing data-sets scenario in machine learning?
- Is there a rule-of-thumb for how to divide a dataset into training and validation sets?