Design and analysis of machine learning experiments

Based on chapter 19 in Alpaydin ML

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Introduction

Managing machine learning

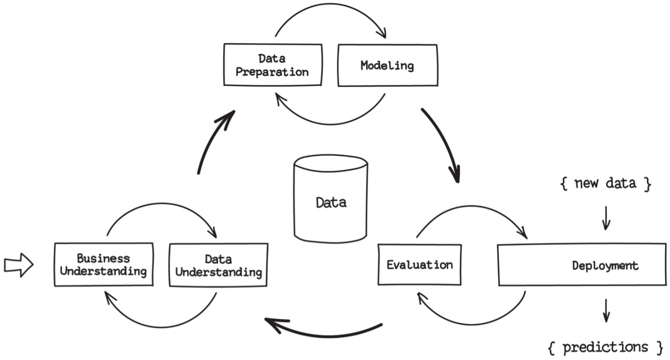
- How confident we are on the error of a model on a dataset?
- How can we compare several methods output on a dataset?
- **Memorizing vs learning**: training - validation - test

Randomness

- Training - validation - test: sampling from data .ipynb
- Model initialization: e.g., with different initial weights, gradients in MLP converge to different local minima
- **Solution: Generalization**
- Average over randomness: use the same algorithms and generate multiple learners, test learners on several validations $\longrightarrow$ distribution over errors (average and scale)

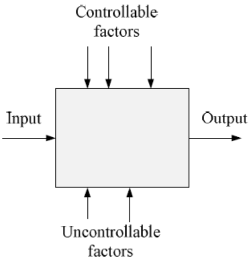
ML process

- ~~**Best algorithm**~~ : Learner is conditioned on dataset
- Training set: optimize parameters
- Validation set: optimize hyperparameters
- Test set: evaluation
- More on model parameter/hyperparameters



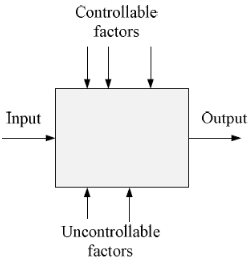
Pictures from towardsdatascience.com

Factors and responses



Factors : algorithms, training set, selected features, etc
Observe the change in response to extract information
Aim : identify important factors and optimize the response

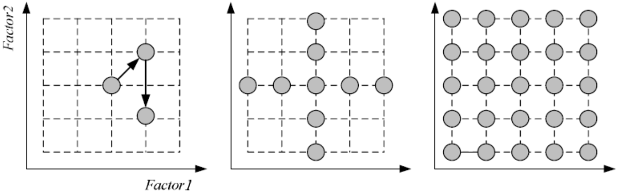
Factors and responses



- Best response based on output
- Source of the randomness: uncontrollable factors (noise in the data, randomly sampling training/validation/test sets and randomness in the optimization process) .ipynb
- Find the configuration of controllable factors that maximizes response and minimally affected by uncontrollable factors

Factor space

How to search the factor space?



(a) Best guess (b) One factor at a time (c) Factorial design

(a) No systematic search and criteria to stop
(b) Assumption: no correlation between factors (often not true)
(c) Grid search: checking all parameter combinations based on a given model - computationally expensive

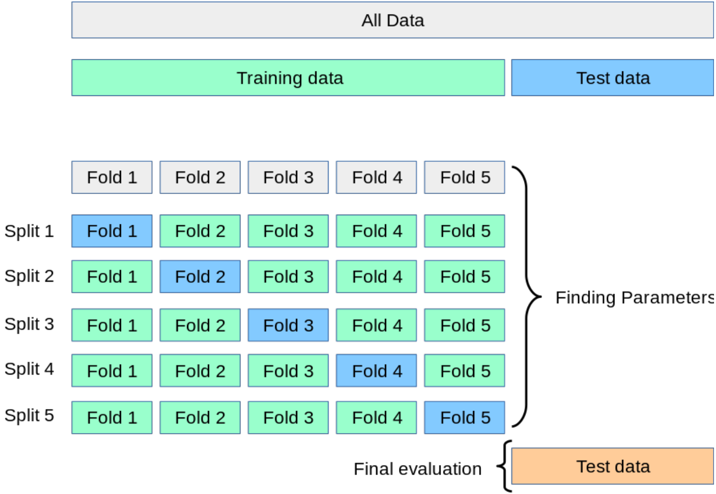
Use knowledge gathered from previous runs that shown a better response. Define a range for hyperparameters and generate random sets of their combinations for random search

Guidelines for ML experiments

- **Aim of the study:** ask correct question
- **Selection of the response variable** (MSE, BC)
- **Choice of factors and levels**
- **Choice of experimental design:** Grid search and random search - dividing data into training/testing : small data gives high variance in responses
- **Performing the experiment:** save intermediate results to be able to rerun partially - equal investigation on multiple ML methods
- **Statistical Analysis of the Data:** visual analysis
- **Conclusions and Recommendations:** start small - investigating results for improvement

Cross-Validation and resampling methods

k-fold Cross-Validation



Pictures from scikit-learn.org

5 times 2-fold CV (Dietterich, 1998)

For i in 5:

1. Shuffle X randomly
2. Divide X into $T_{i1} = X_1$ and $V_{i1} = X_2$
3. Replace partitions: $T_{i2} = X_2$ and $V_{i2} = X_1$

We have 10 different sets:

$$
\begin{aligned}
&\text{Set 1}: T_{11} = X_1 \quad V_{11} = X_2 \\
&\text{Set 2}: T_{12} = X_2 \quad V_{12} = X_1 \\
&\text{Set 3}: T_{21} = X_1' \quad V_{21} = X_2' \\
&\vdots \\
&\text{Set 9}: T_{51} = \hat{X}_1 \quad V_{51} = \hat{X}_2 \\
&\text{Set 10}: T_{52} = \hat{X}_2 \quad V_{52} = \hat{X}_1
\end{aligned}
$$

- With more than 5 iterations: sets share many instances and overlap so much that validation error become too dependent and do not add new information

Bootstrapping

Sampling from a data with replacement. Best way to do resampling for very **small** satasets.

Data = $[1, 2, 3, 4, 5]$
3 samples with size 4 with replacement:

- $s_1 = [1, 2, 3, 3]$
- $s_2 = [5, 1, 5, 3]$
- $s_2 = [3, 4, 3, 5]$

The best way to use bootstrapping is to repeat it several times to get a distribution of the responses.

Performance measurments

Binary classification

		Predicted		
		Positive	Negative	Total
True	Positive	TP (# of TPs)	FN (# of FNs)	p
	Negative	FP (# of FPs)	TN (# of TNs)	n

Confusion matrix for binary classification.

- **Error rate** $= \frac{FP+FN}{p+n}$
- **Accuracy** $= \frac{TP+TN}{p+n}$
- **Sensitivity (recall)** $= \frac{TP}{p}$
- **Specificity** $= \frac{TN}{n}$
- **Precision (Positive predictive value)** $= \frac{Tp}{TP+FP}$
- **False positive rate** $= \frac{FP}{n}$

Example

MNIST digits: one or seven

- Fit a logistic regression to two classes of MNIST digits: one and seven
- After training we evaluate the model with 10 samples of test data.

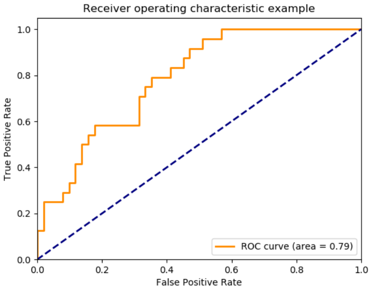
		Predicted		
		one	seven	Total
True	one	4	1	5
	seven	1	4	5

Confusion matrix for binary classification with threshold $= 0.5$

ROC and AUC

- How about different threshold?
- We can calculate sensitivity and specificity for any threshold $\in [0, 1]$.

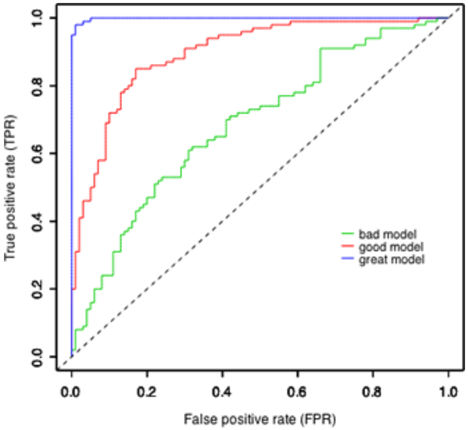
With different classification threshold, instead of using several confusion matrices, we can use ROC (Receiver Operator Characteristic) graphs and AUC (the area under the curve) that show the results in a single easy to interpret graph.



- Diagonal blue line : TP-rate = FP-rate
- X-axis = 1- specificity
- Y-axis : sensitivity
- Compare multiple models with their AUC

Pictures from scikit-learn.org

Model comparison



Pictures from medium.com/usf-msds/