Advanced Machine Learning - Assignment 5

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Introduction

The objective of this assignment is to use the SMBO models to find the hyperparameters of a Multi Layer Perceptron which maximizes the accuracy on a 10 folds cv. The language used in this assignment is python with the SMAC package for the Hyperparameter optimization and Sklearn for the MLPerceptron. Actually there is another easier package based on SMAC called 'auto-sklearn', but in this assignment the basic SMAC package was used. The dataset has 9 features and 1 target, the 9 features are apparently numeric, but the documentation explains that the variable V1 represents the Season and it assumes the following values: -1:'winter', -0.33:'spring', 0.33:'summer', 1.0:'fall', since it is a cyclic variable it cannot be considered completely correct to use ordered variable from -1 to $+1$, thus a one hot encoding is performed, another variable which cannot be considered equidistantly ordered is the V7 (Frequency of alcohol consumption), V7 assumes the following 5 values: 0.2:'several times a day', 0.4:'every day',0.6:'several times a week', 0.8:'once a week',1.0:'hardly ever never', a one hot encoding is also performed in this case.
This is the only basic preprocessing done on the data, the other values were accepted as numeric since they had mostly 2 or 3 classes and were already normalized.

SMAC

The first step is to create a small function around the SMAC package, just for our task (so it won't generalize easily to other problems), this made the code easier for all the exercise. The function is named "optimizer" and it takes in

input the surrogate model name ('rf', 'gp') and will create SMAC4BO for the 'gp' model and SMAC4HPO for the 'rf' model, a configuration space object containing information regarding, the objective function which needs to be minimized, an acquisition function name which can be 'EI', 'LCB' or 'PI', the number of iterations and the number of initial points and an eventual seed.
The optimizer function creates every object necessary for SMAC: Scenario, AcquisionFunction, SMAC Objects etc., the code is commented in a very detailed way[1], the optimizer function return an optimized SMAC object with it's history. The function uses RandomConfigurations to create the initial design, and it hereditates the seed from the SMAC object, so fixing the seed generates the same initial points so all the SMAC models with the same number of initial point will have the same performance on the initial points. A seed (123456789) is fixed for most of the randomness for reproducibility, so the model can be considered deterministic. The objective function in SMAC can only be minimized so instead of weighted accuracy, $1-$ weighted accuracy is used. The other approach for initial points is to generate some random points from the configuration space object and use them as initial points for each model (in case one doesn't want to use seeds).

First Exercise

For the first exercise a Configuration Space is created and it consists of two parameters the 'learning_rate_init' with range between 0.01 and 0.1 and 'momentum' with range between 0.1 and 0.9, the metric used is an weighted accuracy, the weights of each class are the relative frequency of the other class, so the class 'Normal' has a weight of 0.12 and the class 'Altered' (the rare one) has a weight of 0.88, this choice tackles the class imbalance problem with such a low number of data which, since such small number of data makes the oversampling technique somehow problematic.
The 'GP' surrogate model (SMAC4BO) is chosen for this part, and the acquisition functions 'EI', 'LCB' and 'PI' are used with 5 initial points, and the iterations are set to $25 (20 + 5$ initial).
For the GridSearch evenly distributed points are taken from the Configuration Domain (5 for each parameter), and RadomSearch searches random points by itself.

[1] Well surely better than the SMAC documentation.

The MultiLayer perceptron classifier has two hidden layers with 4 and 2 neurons respectively and all the other configuration are the default one, except for the seed which is fixed to have consistent results. In the table 1 the result of the different acquisition function and models[2] are reported. Even though SMAC minimized the error, the weighted accuracy is used to write down the scores and create plots to make them more intuitive.

Acquisitions/Models→	LCB	EI	PI	Random	Grid
Time(seconds)	85.97	95.13	90.30	7.11	7.24
Score(weighted accuracy)	0.582	0.580	0.580	0.580	0.544

Table 1: Results of the First Exercise

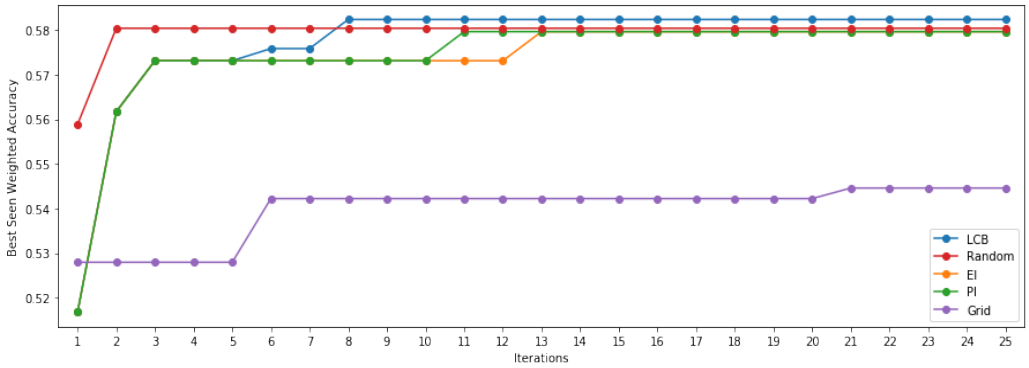


Figure 1: Plot of the result of the First Exercise

From the Table 1 and Figure 1, the best performance is obtained by the GP model with LCB as an acquisition function followed by the RandomSearch, which was fortunate enough to find the it's best configuration at the second iteration, the GP model with EI and PI have the same result and their score is very similar to the RandomSearch (it only differs of 0.0008), while the worst performance is obtained by the GridSearch. In the Figure 1 all the GP model have the same starting point while Grid and Randomized Search starts at different initial points. The best configuration found is with a learning rate of 0.06690282 and a momentum 0.20195706 and in the Table 2 its performance on a 10-CV is reported.

[2]The time values might differ a little in different runs because of the usual small randomnesses in the execution time, while the score should be consistent thanks to the seed.

Metrics	F1	Precision	Recall	F1 Macro	Accuracy
Score	0.173	0.133	0.250	0.536	0.823

Table 2: Results of 10-CV of the Best Configuration for the First Exercise

Second Exercise

The surrogate model is changed to the RandomForest (SMAC4HPO). Two more hyperparameters are added to the configuration space, the number of neurons of the first and second hidden layer, both with a range between 1 and 5, 10 random initial points are chosen and the number of iteration is increased to $110(100 + 10$ initial). The Random and Grid models are used too, in the latter cases the two configurations for the hidden layer size is merged into a single configuration called hidden layer size and it is a tuple of 2 numbers ranging both from 1 to 5.
While for the Random configuration obtaining 110 iterations is easy, for the Grid Search 5 parameters from each configuration is chosen (5 for the learning rate, 5 for the momentum and 5 for the hidden layer sizes) obtaining 125 iterations, for the plot only the last 110 iterations are considered (just to make sure each algorithm has the same length for aesthetics).

Acquisitions/Models→	LCB	EI	PI	Random	Grid
Time(seconds)	210.00	210.06	213.81	24.21	23.90
Score(weighted accuracy)	0.601	0.645	0.601	0.614	0.594

Table 3: Results of the Second Exercise

From the Table 3 and Figure 2 the best algorithm is the RandomForest with EI as acquisition function, improving the weighted accuracy from 0.58 (of the first exercise) to 0.645 with a learning rate of 0.01269289 and momentum of 0.73176491 and with 2 neurons in both layers, in Table 4, it's performance on a 10-CV with other metrics is reported as well, the metric of our interest accuracy is now 0.911, which is better than the zeroRule model[3]. This result should not be surprising since it is known that EI is able to explore and still be able to exploit the information it has. The PI can be expected to fall in a local minima(maxima), but also the LCB was unable to

[3]Trying to maximize the accuracy the optimizer converges to a ML model following a ZeroRule.

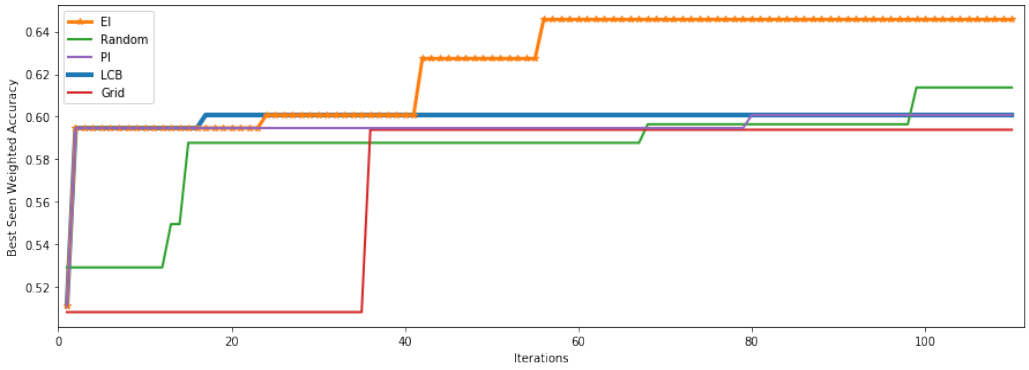


Figure 2: Plot of the result of the Second Exercise

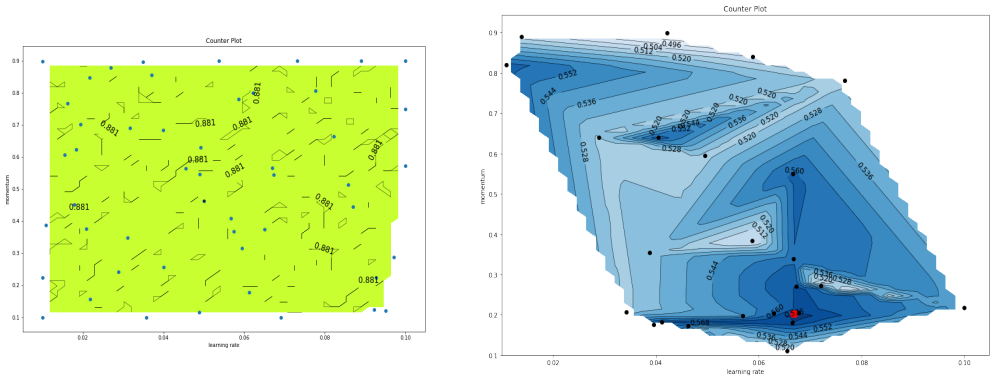
find a better solution for a long number of iterations.
The Random and Grid Search model given more iteration outperforms the models in the First Exercise but requires less time, which is due to the fact that the points in Grid and Search does not depend from other chosen points, thus the calculation can be parallelized completely, in this case the computation was done on a 8 core computer, while the SMBO model needs to wait for the computation of a single configuration to decide the next one, there is an option to parallelize different algorithm in a cluster using 'shared_model' option in scenario Object of SMAC, an algorithm doesn't need to recompute the result of a a configuration that has already been tested on a different algorithm on another machine of the cluster, so using SMAC not in cluster is not really beneficial (for the parallelization).

Metrics	F1	Precision	Recall	F1 Macro	Accuracy
Score	0.300	0.300	0.300	0.626	0.911

Table 4: Results of 10-CV of the Best Configuration for the Second Exercise

Conclusions

One of things than can be noticed using GP as a surrogate model on the second exercise is that GP is about 5× slower than the RF in this case taking nearly 1044 seconds while RF took only about 210 seconds.
The choice of a different metric than the one asked by the assignment is, as



(a) accuracy measure

(b) weighted accuracy

Figure 3: Contour Plot using accuracy and weighted accuracy in the First Exercise with the LCB acquisition function.

already mentioned, due to the class imbalance problem, but another motive is the fact that minimizing the requested metric 'accuracy' with SMBO always made SMBO models to converge to the ZeroRule model, and being to be unable to find a better point of convergence (See Figure 4), some of the reasons are the lack of sufficient data and such a big number of folds in the cross validation, in fact, in each fold the model has at most 1 or 2 elements of the rare class in the test set, if it makes an error on that one the ML model has no more chance on improving its result, while using the weighted accuracy, more weight is given to the rare element, so the MLP is more attentive to that class, and it has the advantage that it does not neglect the non rare class.

In the Figure 3 one can also note how in the case of accuracy the linear interpolation of the evaluated points is flat and the points are being selected randomly, while in the case of weighted accuracy the weighted accuracy function (of learning rate and momentum) is not completely a plateau and the points are clustered at a low value of momentum (the learning rate doesn't seem to change the value too much one of the motive might be that taking a low value of learning rate the model only need more iterations to converge but it will eventually converge to the same point (given the same momentum), the best point is indicated with a red color.

From the results of the second exercise it is clear that improving the model on weighted accuracy it a better choice, as it improves a lot also the accuracy,

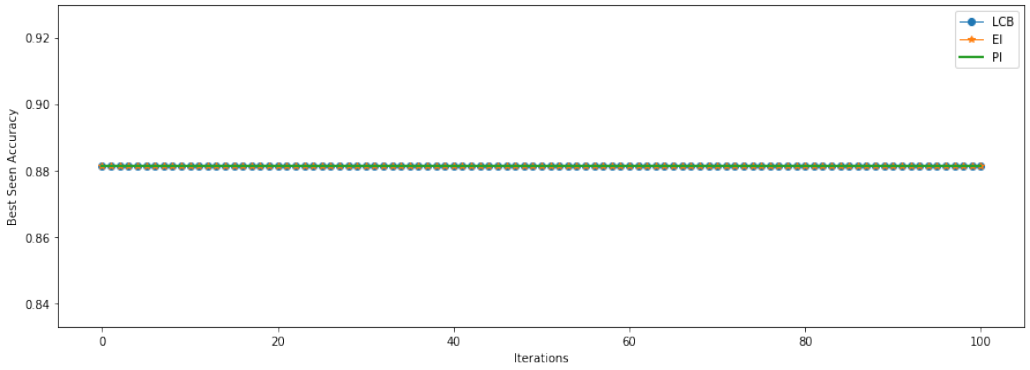


Figure 4: Plot of result with accuracy as measure

which was the objective of this assignment. In the first exercise the model is not able to achieve a better result, due to less parameters that were being optimized and the low number of iterations.
The Grid Search is always outperformed by the other models, while surprisingly (or rather randomically) the Random Search has proved to be a good model, being able to obtain decent performances in both exercises (it is the second best model on both exercises), this was a simple case with a low dimensional hyperparameter space. While the GridSearch doesn't scale well with the high dimensional spaces, the power of RandomSearch is to able to parallelize completely it's computation while it's randomness can be controlled in certain way using some more sophisticated sampling techniques for example the Quasi-Random models to match a more uniform distribution (Sobol, Latin Hypercube). In this simple optimization problem the RandomSearch was able to complete the same number of configurations in 10× less time than the SMBO(because the model evaluation was not expensive), while using just one machine with 8 cores, while to parallelize a SMBO model with Bayesian Optimization with the methodologies used means executing more algorithms, for example using different surrogate models and different acquisition functions, in parallel which shares the Machine Learning Model behavior history in a shared memory. Another great way to parallelize is dividing the hyperparameter space in hyperrectangles, and use SMBO on each space independently, this approach is also knows as DIRECT(DIvide in RECTangles) and it also helps to escape local minima(maxima).