

Simple metafeatures:	Statistical metafeatures:
number of patterns	min # categorical values
log number of patterns	max # categorical values
number of classes	mean # categorical values
number of features	std # categorical values
log number of features	total # categorical values
number of patterns with missing values	kurtosis min
percentage of patterns with missing values	kurtosis max
number of features with missing values	kurtosis mean
percentage of features with missing values	kurtosis std
number of missing values	skewness min
percentage of missing values	skewness max
number of numeric features	skewness mean
number of categorical features	skewness std
ratio numerical to categorical	
ratio categorical to numerical	PCA metafeatures:
dataset dimensionality	pca 95%
log dataset dimensionality	pca skewness first pc
inverse dataset dimensionality	pca kurtosis first pc
log inverse dataset dimensionality	
class probability min	Landmarking metafeatures:
class probability max	One Nearest Neighbor
class probability mean	Linear Discriminant Analysis
class probability std	Naive Bayes
	Decision Tree
	Decision Node Learner
	Random Node Learner
Information-theoretic metafeature:	
class entropy	

Table 1: List of implemented metafeatures

For each dataset, metafeatures are only computed on the training set. In our experiments, for each dataset this required less than one minute and less than the average time it took to evaluate one hyperparameter configuration on that dataset.

Application to Machine Learning Algorithms

We now discuss the machine learning algorithms and their hyperparameters we optimized, as well as the datasets we used in our experiments.

ML Algorithms and Hyperparameters

We empirically evaluated our MI-SMBO approach to optimize two practically relevant machine learning frameworks.

We focused on supervised classification because it is the most widely studied problem in metalearning, with a large body of literature and readily available metafeatures and datasets.²

The large configuration space for our main experiment is spanned by a range of machine learning algorithms from scikit-learn (Pedregosa et al. 2011). We combined all algorithms into a single hierarchical optimization problem using the Combined Algorithm Selection and Hyperparameter optimization (CASH) setting by Thornton et al. (2013): we used

²We note, however, that in principle, our procedure is applicable to every optimization problem that is concerned with minimizing a measurable objective and has a set of metafeatures describing the problem. For example, one possible use in the field of unsupervised learning could be representation learning, with reconstruction error as the objective.

Component	Hyperparameter	Values	# Values
Main	$\theta_{\text{classifier}}$	{RF, SVM, LinearSVM}	3
Main	preprocessing	{PCA, None}	2
SVM	$\log_2(C)$	{-5, -4, ..., 15}	21
SVM	$\log_2(\gamma)$	{-15, -14, ..., 3}	19
LinearSVM	$\log_2(C)$	{-15, -14, ..., 15}	21
LinearSVM	penalty	{ L_1, L_2 }	2
RF	min splits	{1, 2, 4, 7, 10}	5
RF	max features	{1%, 4%, ..., 100%}	10
RF	criterion	{Gini, Entropy}	2
PCA	variance to keep	{80%, 90%}	2

Table 2: Hyperparameters for the CASH problem in scikit-learn. All hyperparameters except $\theta_{\text{classifier}}$ and preprocessing are conditional. Hyperparameters not mentioned were set to their default value.

one top-level hyperparameter $\theta_{\text{classifier}}$ for choosing between classification algorithms, and set all hyperparameters of classification algorithm A_i as conditional on $\theta_{\text{classifier}}$ being set to A_i . This CASH problem is of high practical relevance since it describes precisely the problem an end user faces when given a new dataset.³ To keep the computation bearable and the results interpretable, we only included three classification algorithms: an SVM with an RBF kernel, a linear SVM, and random forests. Since we expected noise and redundancies in the training data, we also allowed the optimization procedure to use Principal Component Analysis (PCA) for preprocessing; with the number of PCA components being conditional on PCA being applied. In total this lead to 10 hyperparameters, as detailed in Table 2. We discretized these 10 hyperparameters to obtain a manageable number of 1 623 hyperparameter configurations that allowed the exhaustive precomputation of classification errors for the entire grid.

We performed a second experiment to test the suitability of our method for a low-dimensional hyperparameter optimization problem: optimizing the complexity penalty C and the kernel width γ of an SVM using an RBF kernel. As above, we discretized these two hyperparameters to a grid of $19 \cdot 21 = 399$ combinations; these constitute a subset of the configurations considered in the CASH problem above.

Datasets and Preprocessing

For our experiments, we aimed for a large number of high-quality classification datasets. We found the OpenML project (Vanschoren et al. 2013) to be the best source of datasets and used the 60 classification datasets it contained in April 2014. For computational reasons we had to exclude three datasets, leaving us with a total of 57. We first shuffled each dataset and then split it in stratified fashion into 2/3 training and 1/3 test data. Then, we computed the validation performance for Bayesian optimization by ten-fold crossvalidation on the training dataset.

To use the same dataset for each classification algorithm,

³We note the existence of previous work on CASH variants for scikit-learn (Hoffman, Shahriari, and de Freitas 2014; Komer, Bergstra, and Eliasmith 2014).

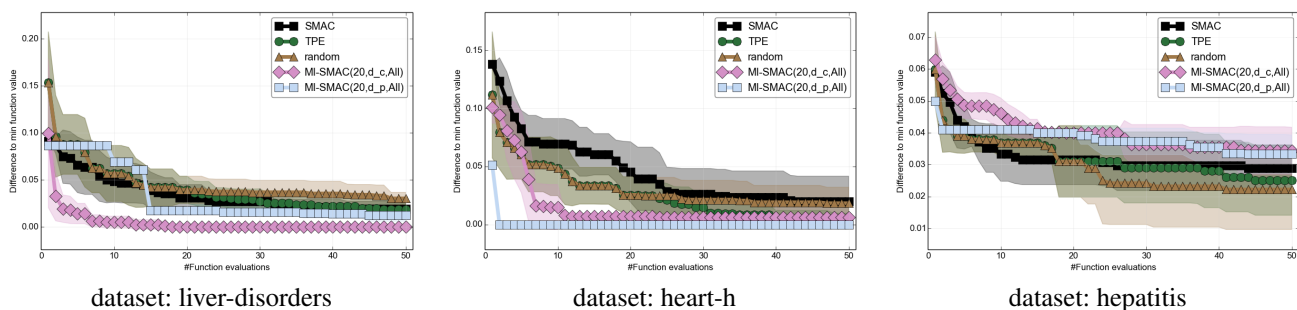


Figure 1: Difference in validation error between hyperparameters found by SMBO and the best value obtained via full grid search for three datasets with scikit-learn. (20, d , X) stands for MI-SMAC with an initial design of $t = 20$ configurations suggested by meta-learning with distance measure d using metafeatures X .

we coded categorical features using a one-hot (aka 1-in- k) encoding, replacing each categorical feature f with domain $\{v_1, \dots, v_k\}$ by k binary variables, only the i -th of which is set to true for data points where f is set to v_i . To retain sparsity, we replaced any missing values with zero. Finally, we scaled numerical features linearly to the range $[0, 1]$.

Experiments

Experimental Setup

We precomputed the 10-fold crossvalidation error on all 57 datasets for each of the 1 623 hyperparameter configurations in our CASH problem. Because the configurations for the SVM benchmark form a subset of these configurations, the corresponding results were reused for the second experiment. Although the classification datasets were no larger than medium-sized ($< 20\,000$ data points), calculating the grid took up to three days per dataset on a modern CPU. This extensive precomputation allowed us to run all our experiments in simulation, by using a lookup table in lieu of running an actual algorithm.

We evaluated our MI-SMBO approach in a leave-one-dataset-out fashion: to evaluate it on one dataset, we assumed knowledge of the other 56 datasets and their best hyperparameter settings. Because Bayesian optimization contains random factors, we repeated each optimization run ten times on each dataset. In total, we thus executed each optimization procedure 570 times.

Our meta-learning initialization approach has several free design choices we had to instantiate for our experiments. These are: the distance metric d , the used metafeatures (we experimented with several subsets suggested in the literature (Pfahringer, Bensusan, and Giraud-Carrier 2000; Bardenet et al. 2013; Yogatama and Mann 2014)) and the number $t \in \{5, 10, 20, 25\}$ of configurations used for initializing SMBO. In total, we evaluated 40 different instantiations of our meta-learning procedure. Due to space restrictions, we only report results for the best of these instantiations; for more results, please see the supplementary material: www.automl.org/aaai2015-mi-smbo-supplementary.pdf

Concerning distance measures, we found the results with d_p and d_c distance to be qualitatively similar, with slightly better results for the d_c measure. We thus restrict the plots

to d_c in several experiments to avoid clutter in the plots. Our experiments with different metafeatures showed that there is no general best set of metafeatures; thus, we only report results using all metafeatures.

Warmstarting SMAC for Optimizing scikit-learn

We now report our results for solving the CASH problem in scikit-learn. First, we evaluated the base performance of the hyperparameter optimization procedures random search, TPE, and SMAC (note that for TPE the prior distributions were uniform) on all 57 datasets and then added meta-learning-initialization to the best of these. Due to the conditional hyperparameters in the scikit-learn space we excluded Spearmint, which – without modification – is known to perform poorly in their presence (Eggenberger et al. 2013).

Figure 1 presents the qualitative performance of all optimizers on three representative datasets. The plots show the mean of the best function values for one optimizer obtained up to a given number of function evaluations. Overall, we found SMAC to outperform both TPE and random search for this large hyperparameter space, confirming the results of Eggenberger et al. (2013). We thus applied our meta-learning initialization to SMAC, but would also expect TPE to benefit from it.

Figure 1 also compares qualitative results of MI-SMAC to the three baselines. In the left plot, the meta-learning suggestions were reasonable and thus lead to MI-SMAC successively improving them over time. In the middle plot the second configuration suggested by meta-learning was already the best, leaving no room for improvement by SMAC. The right plot highlights the fact that meta-learning can also fail and decrease SMAC’s performance.

Next, we analyzed MI-SMAC’s performance using the same ranking-based evaluation as Bardenet et al. (2013) to aggregate over datasets. For each dataset and each function evaluation, we computed the ranks of the three baselines and the two MI-SMAC variants. More precisely, since we had 10 runs of each of the five methods available for each dataset (which give rise to 10^5 possible combinations), we drew a bootstrap sample of 1000 joint runs of the five optimizers and computed the average ranks across these runs. We then further averaged these average ranks across the 57 datasets and show the results in Figure 2. We remind the reader that the rank

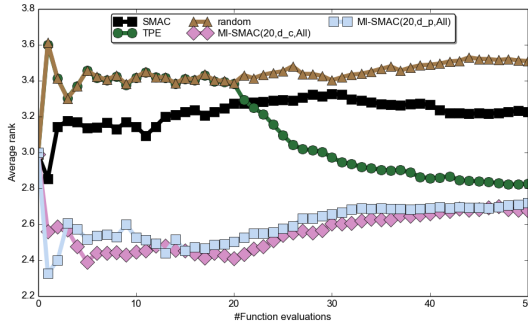


Figure 2: Ranks of various optimizers averaged over all datasets for the CASH problem in scikit-learn.

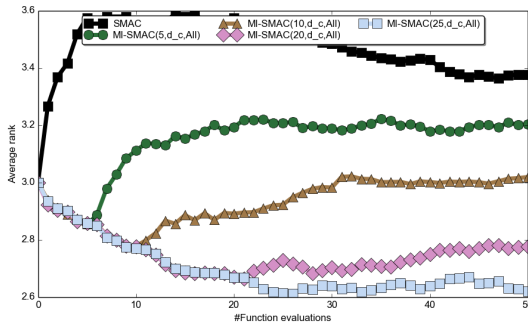


Figure 3: Ranks of SMAC and various MI-SMAC variants averaged over all datasets for the CASH problem in scikit-learn.

is a measure of performance *relative* to the performance of the other optimizers; thus, a method’s rank can increase over time (with larger function evaluation budgets), even though its error decreases, if the other methods achieve greater error reductions. Furthermore, we note that the ranks do not reflect the magnitude of the difference between raw function values.

As Figure 2 shows, the two variants of MI-SMAC performed best, converging to similar ranks with larger function evaluation budgets; and meta-learning yielded dramatically better results for very small function evaluation budgets. We also note that even after 50 function evaluations no SMBO method had fully caught up to the MI-SMBO results. This indicates that meta-learning initialization provided not only good performance with few function evaluations but also a good basis for SMAC to improve upon further.

To demonstrate the effect of varying the number of initial configurations t selected by meta-learning, we plotted the ranks of different instantiations of MI-SMAC in Figure 3. We observe that within the range of t we studied MI-SMAC performs better with more initial configurations.

To complement the above ranking analysis, Figure 4 (top) quantifies on how many datasets MI-SMAC with a learned distance performed significantly better than the other methods according to a two-sided t-test, while Figure 4 (bottom) shows

the statistically significant losses. Both of these quantities are plotted over time, as the function evaluation budget increases.

Compared to the optimizers without meta-learning, MI-SMAC performed much better from the start. Even after 28% of the datasets (in 11% worse), better than SMAC on 35% of the datasets (in 7% worse), and better than random search on 43% of the datasets (in 9% worse). We would like to point out that the improvement MI-SMAC yielded over SMAC is larger than the improvement that SMAC yielded over random search (in 20% better). We attribute this success to the large search space for this problem, which not even SMAC can effectively search in as little as 50 function evaluations. Leveraging successful optimizations from previous datasets clearly helped SMAC in this complex search space.

Warmstarting Spearmint for Optimizing SVMs

To test the generality of our approach we performed an additional experiment on a lower dimensional problem; optimizing the hyperparameters of an SVM on all 57 datasets using Spearmint. We expected Spearmint to yield the best results for this problem as it is known to perform well in cases where the hyperparameters are few and real-valued (Eggenberger et al. 2013). A statistical analysis using a two-sided t-test on the performances for each of the 57 datasets confirms this hypothesis, as Spearmint indeed significantly outperformed TPE, SMAC, and random search in 32%, 44%, and 52% of the datasets, respectively, and only lost in 7%, 8%, and 9% of the cases, respectively.

The ranking plot in Figure 5 shows the performance of Spearmint and two MI-Spearmint variants compared to SMAC, TPE and random search. As this plot shows, the three variants of Spearmint performed best, converging to a similar rank with larger function evaluation budgets. While meta-learning yielded considerably better results for small function evaluation budgets, after about 10 evaluations Spearmint caught up.

As for the scikit-learn benchmark, we also evaluated the effect of using different values of t and plotted these in Figure 6. In contrast to the results for scikit-learn, for this benchmark it was better to use less configurations suggested by meta-learning. In both benchmarks, however, MI-SMBO yielded substantial performance gains over SMBO during the first function evaluations.

Related Work and Possible Extensions

Existing work on using meta-learning for hyperparameter optimization roughly follows two different directions of research. Firstly, Leite, Brazdil, and Vanschoren (2012) developed Active Testing, a method similar to SMBO that reasons across datasets. In contrast to SMBO, Active Testing is a pure algorithm selection method which does not model the effect of hyperparameters (and algorithms) on the results and is limited to a finite number of algorithms. Secondly, meta-learning was used to initialize model-free hyperparameter optimization methods with configurations that previously yielded good performance on similar datasets (Reif, Shafait, and Dengel 2012; Gomes et al. 2012). While similar to our

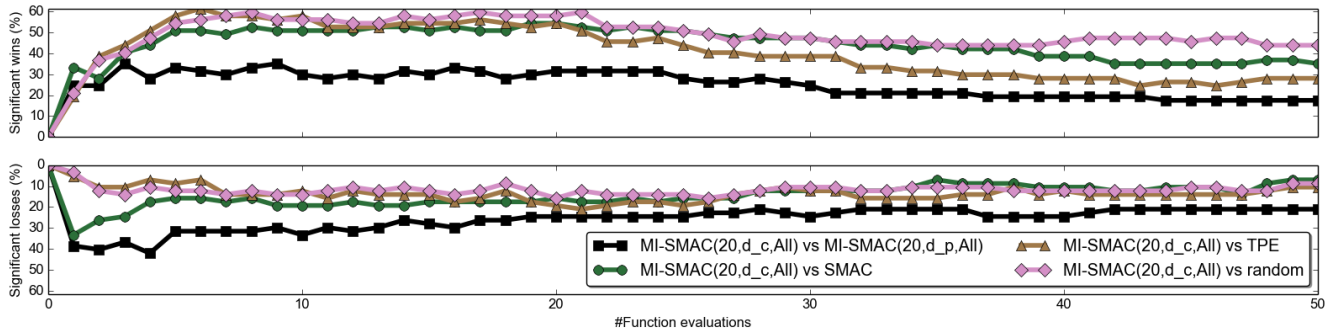


Figure 4: Percentage of wins of MI-SMAC with an initial design of $t = 20$ configurations suggested by meta-learning using the learned distance on all metafeatures. The upper plot shows the number of significant wins of MI-SMAC over competing approaches according to the two-sided t-test while the lower plot shows the statistically significant losses.

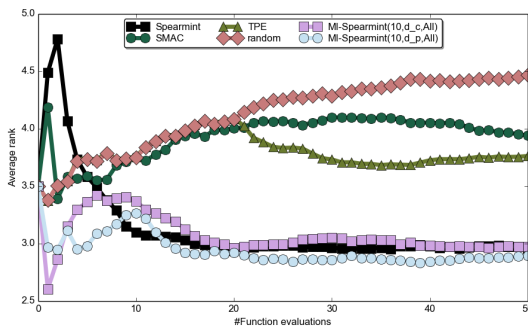


Figure 5: Ranks of various optimizers averaged over all datasets for optimizing the SVM.

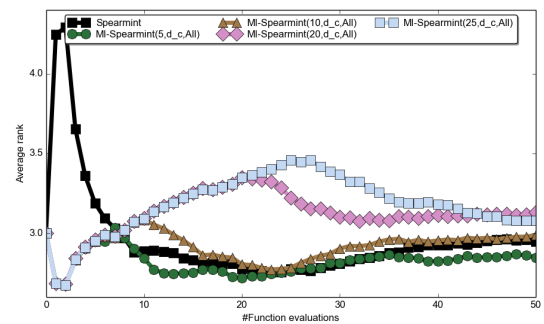


Figure 6: Ranks of Spearmint and various MI-Spearmint variants averaged over all datasets for optimizing the SVM.

work, these methods were limited by their search mechanism and did not improve the state of the art in hyperparameter optimization.

There also exist first attempts to formalize SMBO across several datasets. These collaborative SMBO methods (Bardenet et al. 2013; Swersky, Snoek, and Adams 2013; Yogatama and Mann 2014) address the knowledge transfer directly in the SMBO procedure. However, to date they are limited to small-scale problems with few continuous hyperparameters and a handful of meta-features. In contrast to MI-SMBO they are dependent on the specific SMBO implementation and cannot be readily applied to off-the-shelf hyperparameter optimizers.

Our method’s generality opens several avenues for future work. Here, we evaluated MI-SMBO on small and medium-sized hyperparameter optimization problems, and an important open research question is to extend it to even larger configuration spaces, such as those of Auto-WEKA (Thornton et al. 2013) and Hyperopt-Sklearn (Komer, Bergstra, and Eliasmith 2014). We also plan to extend collaborative SMBO methods to overcome their limitation to small-scale problems. Finally, it would be interesting to extend our work to general algorithm configuration (Hutter, Hoos, and Leyton-Brown 2011) and to the life-long learning setting (Gagliolo and Schmidhuber 2005; Hutter and Hamadi 2005;

Arbelaez, Hamadi, and Sebag 2010).

Conclusion

We have presented a simple, yet effective, method for improving Sequential Model-based Bayesian Optimization (SMBO) by leveraging knowledge from previous optimization runs. Our method combines SMBO with configurations suggested by a meta-learning procedure. It is agnostic of the actual SMBO method used and can thus be applied to the method best suited for a particular problem.

We demonstrated MI-SMBO’s efficacy by improving the initialization of two SMBO methods on a collection of 57 datasets. For a low-dimensional hyperparameter optimization problem, for small optimization budgets MI-Spearmint improved upon the current state of the art algorithm Spearmint. For a large configuration space describing a CASH problem in scikit-learn, MI-SMAC substantially improved over the current state of the art CASH algorithm SMAC (and all other tested optimizers), showing the potential of our approach especially for large-scale hyperparameter optimization.

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