Uncovering Coresets for Classification
With Multi-Objective Evolutionary Algorithms

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Abstract

A *coreset* is a subset of the training set, using which a machine learning algorithm obtains performances similar to what it would deliver if trained over the whole original data. Coreset discovery is an active and open line of research as it allows improving training speed for the algorithms and may help human understanding the results. Building on previous works, a novel approach is presented: candidate corsets are iteratively optimized, adding and removing samples. As there is an obvious trade-off between limiting training size and quality of the results, a multi-objective evolutionary algorithm is used to minimize simultaneously the number of points in the set and the classification error. Experimental results on non-trivial benchmarks show that the proposed approach is able to deliver results that allow a classifier to obtain lower error and better ability of generalizing on unseen data than state-of-the-art coreset discovery techniques.

1. Introduction

A *coreset* is like a small set of paradigmatic examples: a concept can be more effectively explained to a learner resorting to them than by enumerating a longer list of cases. Such an analogy, however, should not be pushed too far: a coreset in Machine Learning (ML) is more formally defined as the minimal set of training samples that allows a supervised algorithm to deliver a result as good as the one obtained when the whole set is used (Bachem et al., 2017). Traditionally, the process of discovering a coreset consists in pinpointing the minimal subset of the data that is sufficient to achieve such good performances. The definition does not specify what is the task of the algorithm (classification, regression, or other), nor what is the quantitative measure used to evaluate its performances. The relevance of coresets

is manifold: reducing the size of the training set can boost the performance of training, limit the memory requirements; and pinpointing the key elements required may provide an insight on the internal process, helping to explain, if not understand, ML results.

While remarkable contributions to the problem date back to 1960s (M. A., 1960), discovering coresets for a specific ML task is still an open and active research line. Plainly, reducing the number of samples could impair the performance of the ML algorithm, and sometimes even state-of-the-art methodologies may not be able to preserve all the information of the original training set. However, coresets have so many advantages that the reduced quality might be acceptable. Therefore, the problem should be more productively framed as *multi-objective*: minimize the size of the corset and maximize the quality of the final result, and eventually let the user to pinpoint the best compromise of these two conflicting goals. Moreover, as ML algorithms employ different techniques to accomplish the same goals, it is also reasonable to assume that they would need coresets of different size and shape to operate at the best of their possibilities. Starting from these two assumptions, and building on previous works (Barbiero & Tonda, 2019a;b; Barbiero et al., 2019), an Evolutionary Algorithm (EA) for coreset discovery is proposed.

When compared to similar works in literature (Barbiero et al., 2019), the proposed EA improves the state of the art as follows:

- it exploits a new representation of coreset candidates in the EA, making it possible to tackle datasets of larger size;

- it does not require parameter tuning, as all relevant parameters are empirically derived from the size of the dataset.

The proposed approach exploits an Evolutionary Algorithm (EA) to drive the automatic selection of coresets. Preliminary experiments suggest that classifiers trained with such evolved samples are able to generalize better than those trained with the whole set. The rest of paper is organized as follows: a few necessary background elements are reported

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in Section 2, the proposed approach is outlined in Section 3, while Section 4 reports the experimental evaluation, and Section 5 concludes the paper.

2. Background

ML literature reports a number of approaches for the identification of coresets in different scenarios, starting from Forward Stagewise published in the 1966 (M. A., 1960) up to the Greedy Iterative Geodesic Ascent (GIGA) appeared in 2018 (Campbell & Broderick, 2018). Other remarkable contributions to this research include Matching Pursuit (Mallat & Zhang, 1993), Orthogonal Matching Pursuit (Ortho Pursuit) (Pati et al., 1993), Frank-Wolfe (Clarkson, 2010), and Least-angle regression (LAR) (Efron et al., 2004; Boutsidis et al., 2013). The original Frank-Wolfe algorithm applies in the context of maximizing a concave function within a feasible polytope by means of a local linear approximation. In Section 4, we refer to the Bayesian implementation of the Frank-Wolfe algorithm designed for core set discovery. This technique, described in (Campbell & Broderick, 2017), aims to find a linear combination of approximated likelihoods (which depends on the core set samples) that is similar to the full likelihood as much as possible. GIGA is a greedy algorithm that further improves Frank-Wolfe. In (Campbell & Broderick, 2018), the authors show that computing the residual error between the full and the approximated likelihoods by using a geodesic alignment guarantees a lower upper bound to the error at the same computational cost. On the other hand, Forward Stagewise, Least-angle regression, Matching Pursuit and Orthogonal Matching Pursuit were all originally devised as greedy algorithms for dimensionality reduction, but have been later applied to coreset discovery, as this last problem represents the transpose of feature selection, choosing samples instead of features. The simplest of the group is Forward Stagewise, which projects high-dimensional data in a lower dimensional space by selecting, one at a time, the features whose inclusion in the model gives the most statistically significant improvement. Matching Pursuit, on the other hand, includes features having the highest inner product with a target signal, while its improved version Orthogonal Matching Pursuit at each step carries an orthogonal projection out. Similarly, Least-angle regression increases the weight of each feature in the direction equiangular to its correlations with the target signal.

While all the above approaches take the size of the coreset as an input of the problem, recently multi-objective EAs were proposed to determine the best trade-off between final performances and coreset size (Barbiero & Tonda, 2019a; Barbiero et al., 2019). Since the 1990s, Evolutionary Computation (EC) techniques have been used to optimize ML frameworks, demonstrating the possibility to determine semi-optimal topologies or to efficiently train artificial neu-

ral networks (Angeline et al., 1994; Maniezzo, 1994; Frean, 1990). A topic where the use of EC soon appeared promising is feature selection (Vafaie & De Jong, 1992; Kim et al., 2000): as the performance of ML algorithms are quite sensitive to the choice of the features, a smart selection procedure is quite beneficial, and EC allowed to automatize the procedure. Selecting features using the eventual performance of a ML algorithm as fitness function is indisputably related to the problem of selecting training-set elements with the same goal.

EAs are stochastic optimization techniques, loosely inspired by the neo-Darwinian paradigm of natural selection. Candidate solutions (*individuals*) are encoded in appropriate data structures (*genomes*); the algorithm manipulates a set of them (*population*), trying to generate better ones. An evaluation function (*fitness function*) is used to assess the extent to which a individual solves the problem; such value controls the probability that the individual is selected for reproduction and survival. In each discrete step of the algorithm (*generation*), new individual (*offspring*) are first generated using *recombination* and *mutation* (cumulatively called *genetic operators*), then evaluated, and eventually the less fit are discarded. The EA stops when a user-defined threshold is reached, typically a limit on the number of generations.

Among the most successful applications of EC, multi-objective optimization often takes the center stage. Optimization problems with contrasting objectives have no single optimal solution. Each candidate represents a different compromise between the multiple conflicting aims. Yet, it is still possible to search for *optimal trade-offs*, for which an objective cannot be improved without degrading the others. The set of such optimal compromises is called *Pareto front* from the 19th century Italian engineer Vilfredo Pareto. Multi-objective evolutionary algorithms (MOEA) currently represent the state of the art for problems with contradictory objectives, and are able to obtain good approximations of the true Pareto front in a reasonable amount of time. One of the most known MOEAs is the Non-Sorting Genetic Algorithm II (NSGA-II) (Deb et al., 2002), that makes use of a special mechanism to spread candidate solutions on the Pareto front as evenly as possible, with considerable efficiency for problems with few objectives.

Interestingly, conflicting objectives to optimize abound in ML, with models being trade-offs between fitting and complexity, and coresets being compromises between number of samples considered and quality of the final result.

3. Proposed approach

In ML, coresets are defined as a subset of the initial (training) dataset that, used on its own, does not significantly
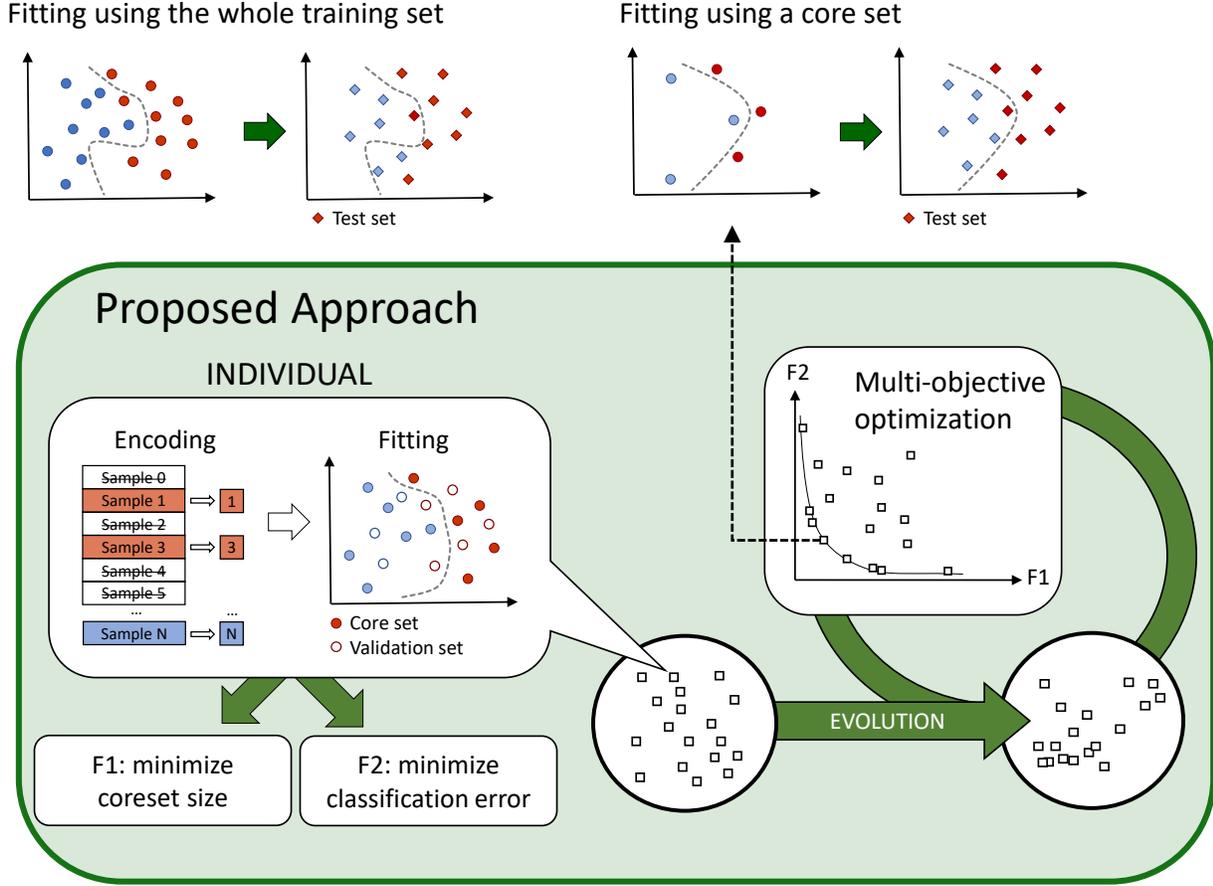
Figure 1. Scheme of the proposed approach. Given a dataset, split into training and test, the original training set is used to seed the initial population with coresets, consisting of sets training samples. Candidate solutions are evaluated on compactness (number of samples) and error (classifier trained on a candidate solution, tested on the original training set). New solutions are obtained through evolutionary operators. Once the evolution is complete, the coresets on the Pareto front undergo a final evaluation, training the classifier that will then compute its error on the (unseen) original test set, to evaluate the generality of the approach.

impact the quality of the results of a ML algorithm with respect to the original dataset. In other terms, coresets can be seen as a *summary* of the information contained in the original dataset, encompassing all the essential data to obtain the correct behavior of the ML algorithm.

As the search space of all possible coresets of varying size for a given problem is clearly vast, it is necessary to resort to stochastic optimization to efficiently explore it. As said before, oreset discovery is inherently a multi-objective problem. Building on previous works on evolutionary coreset discovery (Barbiero & Tonda, 2019a; Barbiero et al., 2019), the proposed algorithm extends and improves the evolutionary approach making it suitable for tackling datasets of larger size without requiring parameter tuning. While the focus of this work is on coreset discovery for classification, it could easily be extended to regression problems. A summary of the proposed algorithm is presented in Figure 1.

The algorithm can be summarized as follows. The dataset $\mathcal{D}$ is split into three groups for training ($\mathcal{D}_t$, 90% of samples), validating ($\mathcal{D}_v$, 10% of samples), and testing ($\mathcal{D}_u$, 10% of samples). Given the training sample $s_i = (\vec{x}^i, y^i) \in \mathcal{D}_t$, where $\vec{x}^i$ is the feature vector of s_i and y^i the corresponding class label, respectively, the objective is to estimate the probability that it belongs to the coreset $\mathcal{C}_j$, given the ML model (i.e., the *classifier*) f:

$$p(s_i \in \mathcal{C}_j | f) \tag{1}$$

Each coreset candidate $\mathcal{C}_j$ is then used to fit the model parameters:

$$p(f_j | \mathcal{C}_j) \tag{2}$$

Finally, the trained classifier is used to make inferences on the training set:

$$p(y_t^i | \vec{x}_t^i, f_j) \tag{3}$$

The proposed approach makes it possible to evolve several solutions $\mathcal{C}_j$ approximating the coreset problem, reducing both the set size and the classification error η:

$$\arg\min_{\mathcal{C}_j} \begin{cases} |\mathcal{C}_j| \\ \eta(f_j, \mathcal{D}_t) \end{cases} \quad (4)$$

The classification error has been defined as 1 minus the weighted F_1 score (Sørensen et al., 1948; Chinchor, 1991) to account for class imbalance in multi-class datasets:

$$\eta = 1 - \frac{1}{\sum_{l \in L} |y_l|} \sum_{l \in L} |y_l| F_1(\hat{y}_l, y_l) \quad (5)$$

where L is the set of labels, $\hat{y}$ the set of *predicted* sample/label pairs, y the set of *true* sample/label pairs, y_l the subset of y with label l, and F_1 given by:

$$F_1 = 2 \times \frac{precision \times recall}{precision + recall} \quad (6)$$

At the end of the evolution, the validation set $\mathcal{D}_v$ is used in order to evaluate the final solutions along the Pareto front. The maximum likelihood estimation for the evolved solutions is given by the core set providing the best score on the validation set:

$$\hat{\mathcal{C}}^{MLE} = \arg\max_{\mathcal{C}_j} 1 - \eta(f_j, \mathcal{D}_v) \quad (7)$$

Finally, $\hat{\mathcal{C}}^{MLE}$ is used to train the model:

$$p(f_{MLE}|\hat{\mathcal{C}}^{MLE}) \quad (8)$$

to make inferences on an unseen test set $\mathcal{D}_u$ and to compute the classification error:

$$\eta(f_{MLE}, \mathcal{D}_u) \quad (9)$$

3.1. Genotype of a candidate solution

The genotype of a candidate solution is represented by a list of integers encoding the position of core samples in the original dataset. The list size may vary for different candidate solutions according to the number of core samples selected.

3.2. Fitness functions

The two fitness functions used in this multi-objective problem are the size of the coreset (to be minimized), and the error of the target classifier trained on core samples, evaluated on the original dataset (to be minimized).

3.3. Population initialization

The starting population of the MOEA is initialized with coresets of random size. The minimum size corresponds to the number of classes in the problem, so that each candidate solution has at least one data point associated to each class; the maximum size is defined as a 1/10 of the original dataset size. Data points in each of such coresets are randomly drawn from the original dataset.

3.4. Evolutionary operators

When generating new candidate solutions, the MOEA randomly selects two individuals and applies the following operators: i. cross over the two candidate solutions, by randomly distributing core samples contained in both between two children solutions; ii. mutate the children solutions adding or removing one sample from their respective list; iii. repair children if the obtained representations violate feasibility constraints (e.g. minimum number of classes, maximum and minimum coreset size).

3.5. Parameters setting

Most parameters in an EA can be derived from a single value, the population size μ. In many practical applications, μ is set through a trial-and-error approach; but there are alternatives, for example the empirical formula used by the state-of-the-art single-objective optimizer Covariance Matrix Adaptation Evolution Strategy (Hansen & Ostermeier, 2001), where population size is determined starting from problem size.

We decided to follow a similar approach, and derive the parameters of the proposed algorithm from the size of the problem, that in the case of coreset discovery can be estimated as 2^k, the total number of possible different coresets of size $[1, k]$, that represents the search space that the algorithm will need to explore in order to find the best coreset candidate. We fix $k = 0.1 * N$, where N is the total number of samples in the considered data set, as in most practical cases desirable coresets are 10% or less of the initial samples.

Following the empirical formulas presented in (Hansen & Ostermeier, 2001), starting from k we can then derive the other necessary parameters for NSGA-II:

$$\mu = \lfloor \max(100, log_{10} 2^k) \rfloor \quad (10)$$
$$\lambda = 2 * \mu \quad (11)$$
$$\mathcal{G} = \lfloor \max(100, log_{10} 2^{k \cdot 0.5}) \rfloor \quad (12)$$

Where μ, as mentioned above, is the size of the population; λ is the size of the offspring, the number of new candidate solutions generated at each iteration; and $\mathcal{G}$ is the number of iterations after which the algorithm will stop. When compared to the empirical formulas of CMA-ES for deriving parameters, the main difference is that we increased the minimum size of the population and the minimum number

of iterations, as the specific problem we are tackling is quite challenging.

4. Experimental Evaluation

All the necessary code for the experiments has been implemented in Python 3, relying upon open-source libraries as `scikit-learn v0.22`[1] (Pedregosa et al., 2011) and `inspyred v1.0`[2] (Garrett, 2012), and `bayesiancoresets v0.8`[3] (Campbell & Beronov, 2019). The code is freely available under GNU Public License from a GitHub public repository[4]. NSGA-II is used with the default parameters set by `inspyred`, with the exceptions described in subsection 3.5. In order to generate reproducible results, all algorithms that exploit pseudo-random elements in their training process have been set with a fixed seed. Before running coreset selection algorithms, each dataset has been standardized removing the mean and scaling to unit variance (`StandardScaler` (Zill et al., 2011)). All the experiments have been run on the same machine: nn AMD EPYC 7301 16-Core Processor at 2 GHz equipped with 64 MiB memory.

Table 1 summarizes the main characteristics of the benchmark datasets used for the experiments. All of them have been downloaded from the OpenML public repository (Vanschoren et al., 2013; Matthias Feurer).

Table 1. Benchmark datasets

DATA SET	SAMPLES	FEATURES	CLASSES	NANS
MICRO-MASS	571	1,301	20	0
SOYBEAN	683	36	19	2,337
CREDIT-G	1,000	21	2	0
KR-VS-KP	3,196	37	2	0
ABALONE	4,177	9	28	0
ISOLET	7,797	618	26	0
JM1	10,885	22	2	25
GAS-DRIFT	13,910	129	6	0
MOZILLA4	15,545	6	2	0
LETTER	20,000	17	26	0
AMAZON	32,769	10	2	0
ELECTRICITY	45,312	9	2	0
MNIST	70,000	785	10	0
COVERTYPE	581,012	55	17	0

The proposed approach has been tested over a 10-fold cross-validation against state-of-the-art coreset discovery

algorithms: GIGA (Campbell & Broderick, 2018), Frank-Wolfe (Clarkson, 2010), Matching Pursuit (Pati et al., 1993), Orthogonal Mathcing Pursuit (Pati et al., 1993), LAR (Efron et al., 2004; Boutsidis et al., 2013), and Forward Stagewise (M. A., 1960). For each fold, coresets have been extracted and used to train an instance of the `Ridge` (Tikhonov, 1943) classifier. This classifier has been chosen both for its high train speed and its generalization ability in a variety of experimental settings. Figures 2 and 3 show for each benchmark dataset the quality of extracted coresets as a function of coreset size (lower is better), and classification error (lower is better). The coreset size has been reported both as the absolute number of core samples (in round brackets) and as the ratio $|\hat{\mathcal{C}}^{MLE}|/|\mathcal{D}_t|$ (number of core samples over the total number of training samples). The error bars represent the standard error of the mean. Details about experimental results are shown in the Table 2 and 3. The results can be summarized as follows:

- Concerning just mean classification error, EvoCore outperformed state-of-the-art techniques on all datasets but two, namely Micro-mass and MNIST;

- Considering coreset discovery as a multi-objective problem (minimize classification error and minimize coreset size), EvoCore's coresets are never dominated by the coresets uncovered by other techniques, for all considered datasets. On the contrary, they often dominate a considerable number of other solutions.

- In most cases, the solution provided by EvoCore was in a region of the search space far away from the solutions provided by the other techniques, thus revealing compromises unexplored by competitors.

When compared to the state-of-the-art in coreset discovery, EvoCore thus proves to be extremely effective. The main drawback of the proposed approach is represented by the longer running time. However, the problem can be mitigated by parallelizing evaluations, as EAs can easily evaluate all individuals in the same generation at the same time, provided that enough computational resources are available.

5. Conclusions

In this work, a novel alternative to coreset discovery is presented. Experimental results suggest that the performance of ML classifiers would not be a function of the *size* of the training set, but rather a function of the *mutual position* of the training samples in the feature space. Future works will explore the possibility of extending coreset discovery to regression and clustering.

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[1]scikit-learn: Machine Learning in Python, http://scikit-learn.org/

[2]inspyred: Bio-inspired Algorithms in Python, https://pythonhosted.org/inspyred/

[3]bayesiancoresets: Coresets for approximate Bayesian inference, https://github.com/trevorcampbell/bayesian-coresets/

[4]GitHub, https://github.com/albertotonda/prototype-set-discovery
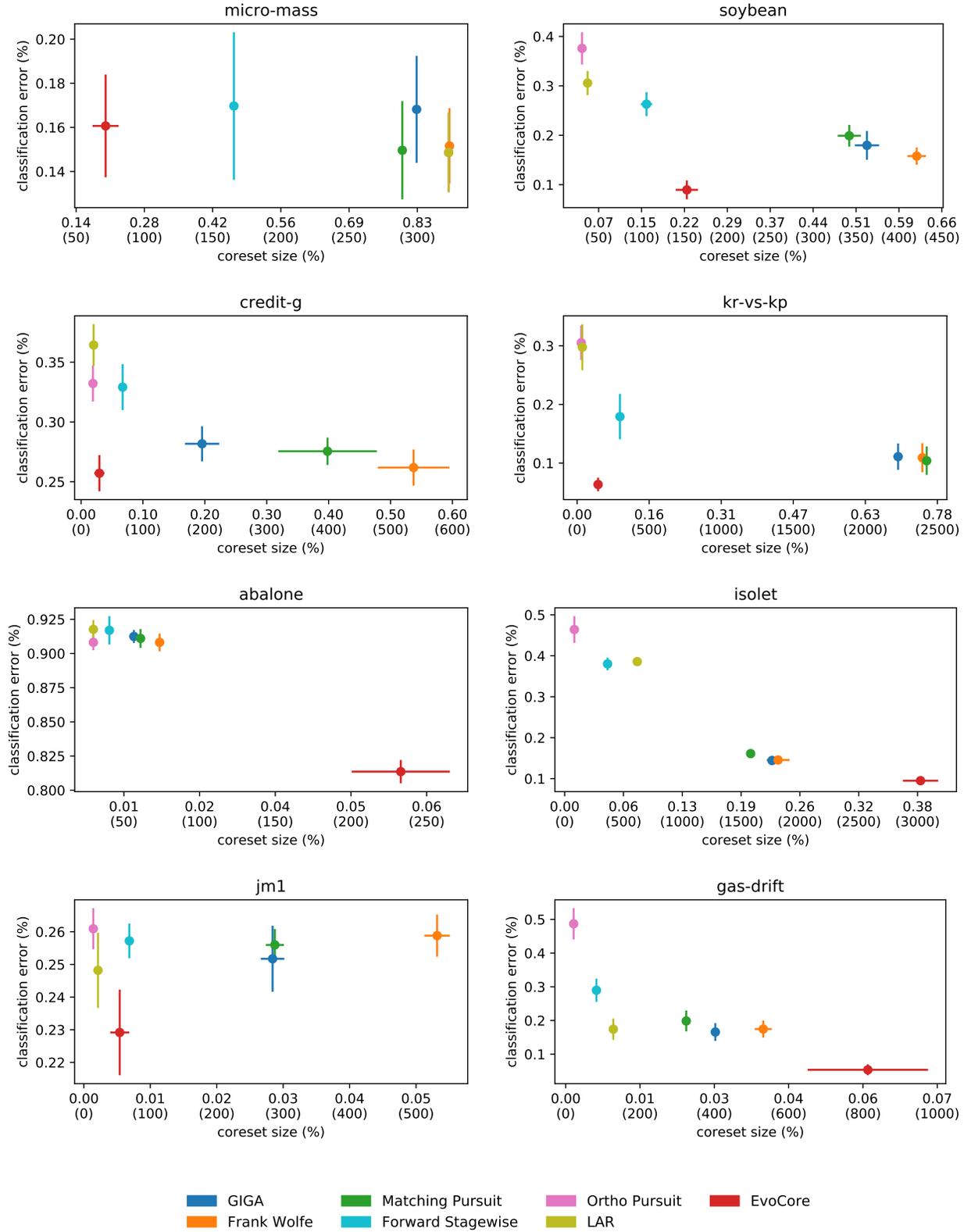
Figure 2. The figures show for each benchmark dataset the quality of extracted coresets as a function of coreset size (lower is better), and classification error obtained using an instance of the `Ridge` classifier (lower is better). The error bars represent the standard error of the mean.
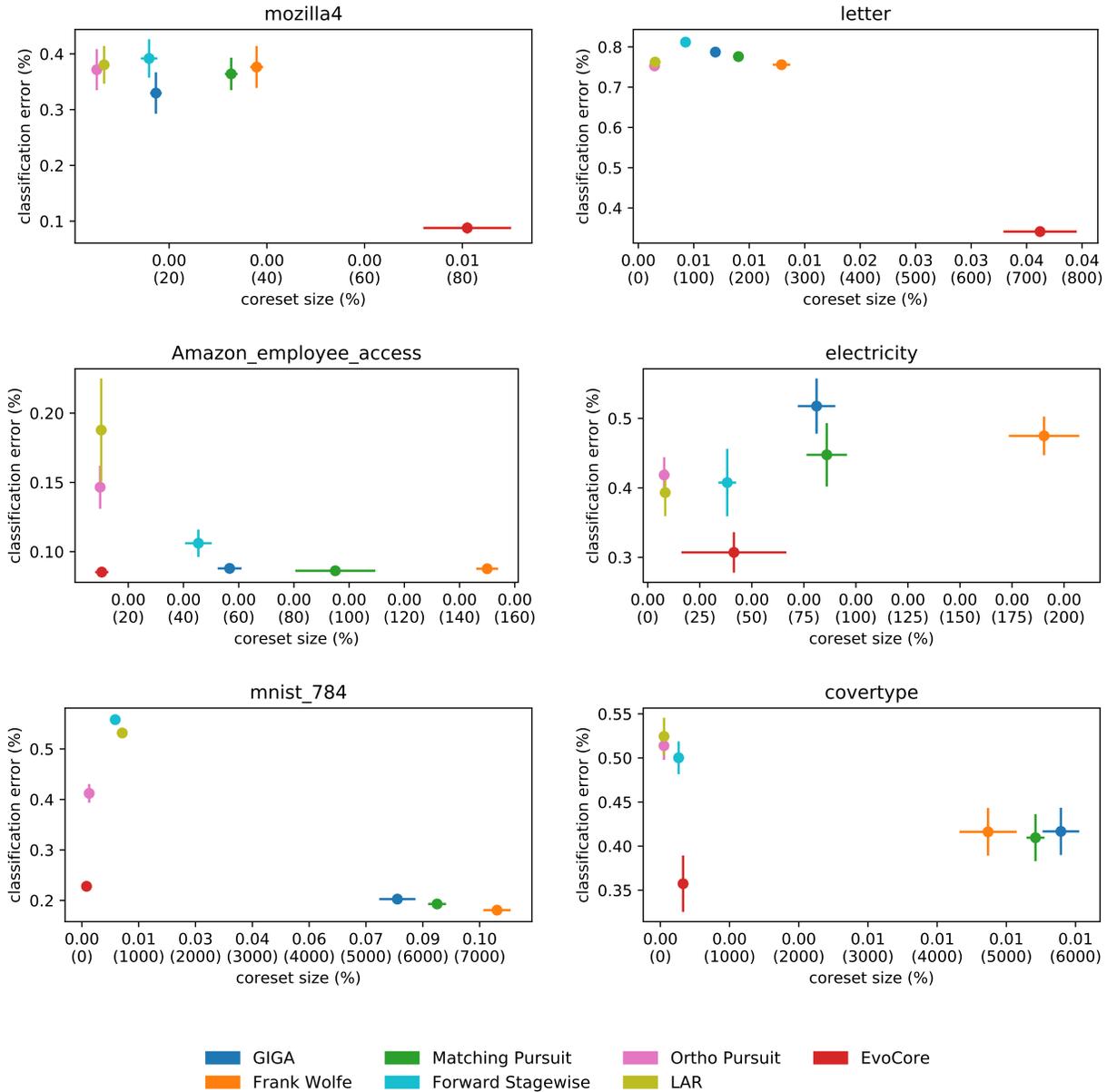
Figure 3. The figures show for each benchmark dataset the quality of extracted coresets as a function of coreset size (lower is better), and classification error obtained using an instance of the `Ridge` classifier (lower is better). The error bars represent the standard error of the mean.

Software and Data

Should this paper be accepted, a link to a repository with all the code needed to reproduce the experiments will be provided.

References

Angeline, P. J., Saunders, G. M., and Pollack, J. B. An evolutionary algorithm that constructs recurrent neural networks. *IEEE transactions on Neural Networks*, 5(1): 54–65, 1994.

Bachem, O., Lucic, M., and Krause, A. Practical coreset constructions for machine learning. *arXiv preprint arXiv:1703.06476*, 2017.

Barbiero, P. and Tonda, A. Fundamental flowers: Finding core sets for classification using evolutionary computation. In *Evostar 2019*, 04 2019a.

Table 2. 10-fold cross-validation results. The mean and the standard error of the mean (s.e.m.) is reported in each column. The result with the best (highest or lowest) mean value for each metric is highlighted in **bold**.

MICRO-MASS	SIZE	TEST F_1	TRAIN F_1	FIT TIME (S)
GIGA	299.50 ± 0.67	0.832 ± 0.024	0.995 ± 0.002	21.80 ± 0.22
FRANK-WOLFE	323.60 ± 0.27	0.848 ± 0.017	1.000 ± 0.000	59.55 ± 0.28
MATCHING PURSUIT	289.00 ± 1.29	0.850 ± 0.022	0.992 ± 0.002	61.40 ± 0.20
FORWARD STAGEWISE	165.60 ± 1.36	0.830 ± 0.033	0.945 ± 0.007	60.49 ± 0.32
ORTHO PURSUIT	323.00 ± 0.00	**0.851 ± 0.018**	1.000 ± 0.000	231.35 ± 139.34
LAR	323.00 ± 0.00	**0.851 ± 0.018**	1.000 ± 0.000	21.84 ± 0.29
EVOCORE	**71.60 ± 9.54**	0.839 ± 0.023	0.968 ± 0.009	227.98 ± 2.95

SOYBEAN	SIZE	TEST F_1	TRAIN F_1	FIT TIME (S)
GIGA	362.70 ± 14.11	0.820 ± 0.029	0.860 ± 0.008	3.56 ± 0.12
FRANK-WOLFE	420.70 ± 10.74	0.842 ± 0.018	0.865 ± 0.012	1.79 ± 0.10
MATCHING PURSUIT	342.10 ± 13.52	0.801 ± 0.022	0.829 ± 0.011	2.34 ± 0.11
FORWARD STAGEWISE	105.80 ± 6.62	0.737 ± 0.024	0.786 ± 0.017	1.94 ± 0.12
ORTHO PURSUIT	30.60 ± 1.50	0.624 ± 0.033	0.680 ± 0.028	0.81 ± 0.19
LAR	37.10 ± 0.35	0.694 ± 0.024	0.717 ± 0.012	**0.80 ± 0.16**
EVOCORE	152.80 ± 12.95	**0.911 ± 0.019**	0.956 ± 0.001	96.87 ± 0.91

CREDIT-G	SIZE	TEST F_1	TRAIN F_1	FIT TIME (S)
GIGA	195.50 ± 27.65	0.718 ± 0.015	0.721 ± 0.005	1.19 ± 0.18
FRANK-WOLFE	537.20 ± 57.91	0.738 ± 0.015	0.739 ± 0.006	1.93 ± 0.07
MATCHING PURSUIT	398.20 ± 79.64	0.724 ± 0.011	0.737 ± 0.006	2.09 ± 0.09
FORWARD STAGEWISE	67.20 ± 1.91	0.671 ± 0.019	0.676 ± 0.011	2.06 ± 0.11
ORTHO PURSUIT	19.20 ± 0.80	0.668 ± 0.015	0.658 ± 0.009	0.63 ± 0.12
LAR	20.30 ± 0.21	0.636 ± 0.017	0.636 ± 0.014	0.67 ± 0.10
EVOCORE	29.60 ± 8.28	**0.743 ± 0.015**	0.773 ± 0.007	124.58 ± 0.92

KR-VS-KP	SIZE	TEST F_1	TRAIN F_1	FIT TIME (S)
GIGA	2227.30 ± 32.20	0.889 ± 0.022	0.939 ± 0.002	4.48 ± 0.22
FRANK-WOLFE	2395.60 ± 16.58	0.891 ± 0.025	0.940 ± 0.001	5.18 ± 0.11
MATCHING PURSUIT	2425.70 ± 19.22	0.896 ± 0.024	0.942 ± 0.002	6.25 ± 0.17
FORWARD STAGEWISE	297.40 ± 24.03	0.821 ± 0.039	0.878 ± 0.011	5.71 ± 0.13
ORTHO PURSUIT	28.70 ± 2.42	0.695 ± 0.029	0.732 ± 0.014	**0.76 ± 0.17**
LAR	36.10 ± 0.18	0.702 ± 0.039	0.743 ± 0.014	0.87 ± 0.16
EVOCORE	145.50 ± 28.12	**0.937 ± 0.012**	0.968 ± 0.001	146.55 ± 0.53

ABALONE	SIZE	TEST F_1	TRAIN F_1	FIT TIME (S)
GIGA	56.60 ± 2.87	0.088 ± 0.005	0.089 ± 0.004	1.69 ± 0.25
FRANK-WOLFE	73.60 ± 2.40	0.092 ± 0.007	0.098 ± 0.004	2.96 ± 0.11
MATCHING PURSUIT	61.00 ± 2.03	0.089 ± 0.007	0.095 ± 0.002	3.13 ± 0.12
FORWARD STAGEWISE	40.40 ± 1.94	0.083 ± 0.010	0.083 ± 0.009	3.32 ± 0.15
ORTHO PURSUIT	29.80 ± 0.49	0.092 ± 0.006	0.096 ± 0.005	1.14 ± 0.26
LAR	29.80 ± 0.47	0.082 ± 0.007	0.090 ± 0.009	1.61 ± 0.61
EVOCORE	232.90 ± 32.43	**0.186 ± 0.009**	0.194 ± 0.003	44.52 ± 0.08

ISOLET	SIZE	TEST F_1	TRAIN F_1	FIT TIME (S)
GIGA	1763.10 ± 13.97	0.856 ± 0.007	0.902 ± 0.002	208.60 ± 0.35
FRANK-WOLFE	1814.50 ± 97.73	0.854 ± 0.005	0.902 ± 0.002	543.19 ± 0.44
MATCHING PURSUIT	1581.20 ± 23.01	0.839 ± 0.006	0.883 ± 0.002	560.61 ± 1.67
FORWARD STAGEWISE	364.90 ± 5.67	0.620 ± 0.015	0.655 ± 0.009	564.02 ± 0.62
ORTHO PURSUIT	82.20 ± 10.12	0.536 ± 0.033	0.559 ± 0.026	6.58 ± 0.89
LAR	617.00 ± 0.00	0.614 ± 0.008	0.659 ± 0.002	433.81 ± 40.76
EVOCORE	3025.50 ± 150.26	**0.905 ± 0.006**	0.952 ± 0.002	7029.46 ± 49.88

JM1	SIZE	TEST F_1	TRAIN F_1	FIT TIME (S)
GIGA	284.10 ± 17.68	0.748 ± 0.010	0.748 ± 0.001	8.33 ± 0.52
FRANK-WOLFE	531.70 ± 19.20	0.741 ± 0.006	0.745 ± 0.002	26.58 ± 0.13
MATCHING PURSUIT	287.50 ± 13.64	0.744 ± 0.005	0.748 ± 0.002	27.25 ± 0.12
FORWARD STAGEWISE	68.50 ± 1.29	0.743 ± 0.005	0.744 ± 0.006	27.61 ± 0.11
ORTHO PURSUIT	14.20 ± 1.21	0.739 ± 0.006	0.745 ± 0.005	**0.87 ± 0.10**
LAR	21.30 ± 0.15	0.752 ± 0.012	0.754 ± 0.003	1.11 ± 0.13
EVOCORE	54.00 ± 14.35	**0.771 ± 0.013**	0.788 ± 0.002	844.78 ± 1.94

Table 3. 10-fold cross-validation results. The mean and the standard error of the mean (s.e.m.) is reported in each column. The result with the best (highest or lowest) mean value for each metric is highlighted in **bold**.

GAS-DRIFT	SIZE	TEST F_1	TRAIN F_1	FIT TIME (S)
GIGA	402.70 ± 6.11	0.834 ± 0.026	0.876 ± 0.016	77.82 ± 0.48
FRANK-WOLFE	531.70 ± 23.01	0.825 ± 0.025	0.886 ± 0.011	195.76 ± 0.21
MATCHING PURSUIT	324.40 ± 8.06	0.801 ± 0.031	0.859 ± 0.017	195.28 ± 0.17
FORWARD STAGEWISE	82.80 ± 3.13	0.710 ± 0.034	0.742 ± 0.025	195.12 ± 0.17
ORTHO PURSUIT	21.40 ± 2.66	0.513 ± 0.046	0.579 ± 0.034	**1.21 ± 0.10**
LAR	128.10 ± 0.10	0.826 ± 0.031	0.887 ± 0.007	20.83 ± 1.15
EVOCORE	813.10 ± 162.08	**0.946 ± 0.016**	0.986 ± 0.001	3517.78 ± 30.70

MOZILLA4	SIZE	TEST F_1	TRAIN F_1	FIT TIME (S)
GIGA	17.30 ± 1.17	0.670 ± 0.037	0.665 ± 0.029	1.04 ± 0.21
FRANK-WOLFE	37.90 ± 1.31	0.624 ± 0.038	0.630 ± 0.035	6.26 ± 0.15
MATCHING PURSUIT	32.70 ± 1.30	0.636 ± 0.029	0.628 ± 0.021	6.46 ± 0.06
FORWARD STAGEWISE	15.90 ± 1.70	0.608 ± 0.035	0.578 ± 0.024	6.39 ± 0.08
ORTHO PURSUIT	5.20 ± 0.20	0.628 ± 0.037	0.604 ± 0.044	**0.96 ± 0.18**
LAR	6.70 ± 0.40	0.620 ± 0.034	0.611 ± 0.025	2.73 ± 1.31
EVOCORE	81.00 ± 8.98	**0.912 ± 0.010**	0.912 ± 0.001	2041.79 ± 4.50

LETTER	SIZE	TEST F_1	TRAIN F_1	FIT TIME (S)
GIGA	139.00 ± 5.31	0.213 ± 0.007	0.215 ± 0.007	1.13 ± 0.12
FRANK-WOLFE	258.20 ± 15.72	0.244 ± 0.008	0.246 ± 0.009	38.61 ± 0.17
MATCHING PURSUIT	180.50 ± 6.80	0.224 ± 0.009	0.227 ± 0.009	39.00 ± 0.14
FORWARD STAGEWISE	85.20 ± 5.90	0.188 ± 0.007	0.192 ± 0.008	39.17 ± 0.12
ORTHO PURSUIT	29.30 ± 0.40	0.247 ± 0.010	0.246 ± 0.009	**0.95 ± 0.11**
LAR	30.30 ± 0.37	0.238 ± 0.007	0.243 ± 0.007	8.54 ± 5.20
EVOCORE	724.30 ± 66.09	**0.659 ± 0.004**	0.669 ± 0.002	6916.12 ± 33.55

AMAZON-EMPLOYEE-ACCESS	SIZE	TEST F_1	TRAIN F_1	FIT TIME (S)
GIGA	56.70 ± 4.33	0.912 ± 0.001	0.912 ± 0.001	1.28 ± 0.23
FRANK-WOLFE	150.00 ± 3.96	0.912 ± 0.001	0.912 ± 0.002	5.18 ± 0.17
MATCHING PURSUIT	95.00 ± 14.50	0.914 ± 0.000	0.914 ± 0.000	39.43 ± 0.21
FORWARD STAGEWISE	45.40 ± 4.84	0.894 ± 0.010	0.894 ± 0.010	39.09 ± 0.16
ORTHO PURSUIT	9.80 ± 0.29	0.853 ± 0.016	0.852 ± 0.015	**0.89 ± 0.28**
LAR	10.20 ± 0.33	0.812 ± 0.037	0.811 ± 0.037	8.73 ± 5.36
EVOCORE	10.40 ± 2.38	**0.915 ± 0.000**	0.915 ± 0.000	14098.09 ± 177.97

ELECTRICITY	SIZE	TEST F_1	TRAIN F_1	FIT TIME (S)
GIGA	81.10 ± 9.03	0.482 ± 0.040	0.513 ± 0.020	1.27 ± 0.18
FRANK-WOLFE	190.40 ± 16.92	0.525 ± 0.028	0.553 ± 0.014	47.35 ± 0.17
MATCHING PURSUIT	86.00 ± 9.74	0.552 ± 0.046	0.553 ± 0.036	47.97 ± 0.14
FORWARD STAGEWISE	38.20 ± 4.29	0.592 ± 0.049	0.618 ± 0.037	47.47 ± 0.14
ORTHO PURSUIT	7.90 ± 0.10	0.581 ± 0.026	0.622 ± 0.027	**0.97 ± 0.14**
LAR	8.40 ± 0.22	0.607 ± 0.034	0.607 ± 0.024	0.99 ± 0.10
EVOCORE	41.40 ± 25.20	**0.693 ± 0.029**	0.759 ± 0.003	38331.78 ± 84.84

MNIST	SIZE	TEST F_1	TRAIN F_1	FIT TIME (S)
GIGA	5552.30 ± 319.09	0.797 ± 0.003	0.807 ± 0.003	**1.41 ± 0.08**
FRANK-WOLFE	7306.20 ± 240.28	**0.819 ± 0.004**	0.826 ± 0.002	3075.35 ± 172.95
MATCHING PURSUIT	6250.90 ± 157.99	0.807 ± 0.004	0.816 ± 0.002	3080.56 ± 128.81
FORWARD STAGEWISE	587.00 ± 5.79	0.442 ± 0.004	0.449 ± 0.005	3009.10 ± 166.47
ORTHO PURSUIT	128.80 ± 20.96	0.588 ± 0.019	0.590 ± 0.018	46.48 ± 5.72
LAR	711.00 ± 0.26	0.468 ± 0.007	0.477 ± 0.005	746.32 ± 41.71
EVOCORE	**82.00 ± 3.86**	0.772 ± 0.006	0.773 ± 0.003	4001.79 ± 157.18

COVERTYPE	SIZE	TEST F_1	TRAIN F_1	FIT TIME (S)
GIGA	5788.40 ± 265.86	0.583 ± 0.027	0.637 ± 0.006	1319.12 ± 121.27
FRANK-WOLFE	4735.80 ± 413.56	0.584 ± 0.027	0.626 ± 0.007	1888.11 ± 99.88
MATCHING PURSUIT	5421.30 ± 129.91	0.590 ± 0.027	0.630 ± 0.007	1893.71 ± 96.84
FORWARD STAGEWISE	264.20 ± 12.45	0.500 ± 0.019	0.533 ± 0.006	1975.60 ± 46.11
ORTHO PURSUIT	52.60 ± 0.22	0.486 ± 0.016	0.501 ± 0.012	17.25 ± 1.44
LAR	53.30 ± 0.21	0.476 ± 0.021	0.505 ± 0.014	29.26 ± 2.52
EVOCORE	328.40 ± 59.92	**0.643 ± 0.032**	0.701 ± 0.003	4881.47 ± 106.46

Barbiero, P. and Tonda, A. Making sense of economics datasets with evolutionary coresets. In *The International Conference on Decision Economics*, pp. 162–170. Springer, 2019b.

Barbiero, P., Squillero, G., and Tonda, A. Evolutionary discovery of coresets for classification. In *Proceedings of the Genetic and Evolutionary Computation Conference Companion*, pp. 1747–1754, 2019.

Boutsidis, C., Drineas, P., and Magdon-Ismail, M. Near-optimal Coresets For Least-Squares Regression. Technical report, 2013. URL https://arxiv.org/pdf/1202.3505.pdf.

Campbell, T. and Beronov, B. Sparse variational inference: Bayesian coresets from scratch. In *Advances in Neural Information Processing Systems*, pp. 11457–11468, 2019.

Campbell, T. and Broderick, T. Automated Scalable Bayesian Inference via Hilbert Coresets. 2017. URL http://arxiv.org/abs/1710.05053.

Campbell, T. and Broderick, T. Bayesian Coreset Construction via Greedy Iterative Geodesic Ascent. In *International Conference on Machine Learning (ICML)*, 2018. URL https://arxiv.org/pdf/1802.01737.pdf.

Chinchor, N. Muc-3 evaluation metrics. In *Proceedings of the 3rd conference on Message understanding*, pp. 17–24. Association for Computational Linguistics, 1991.

Clarkson, K. L. Coresets, Sparse Greedy Approximation, and the Frank-Wolfe Algorithm. In *ACM Transactions on Algorithms*, 2010. URL http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.145.9299{&}rep=rep1{&}type=pdf.

Deb, K., Pratap, A., Agarwal, S., and Meyarivan, T. A fast and elitist multiobjective genetic algorithm: Nsga-ii. *IEEE transactions on evolutionary computation*, 6(2): 182–197, 2002.

Efron, B., Hastie, T., Johnstone, I., and Tibshirani, R. Least Angle Regression. *The Annals of Statistics*, 32(2):407–451, 2004. doi: 10.1214/009053604000000067. URL https://arxiv.org/pdf/math/0406456.pdf.

Frean, M. The upstart algorithm: A method for constructing and training feedforward neural networks. *Neural computation*, 2(2):198–209, 1990.

Garrett, A. inspyred (version 1.0.1) inspired intelligence. https://github.com/aarongarrett/inspyred, 2012.

Hansen, N. and Ostermeier, A. Completely derandomized self-adaptation in evolution strategies. *Evolutionary computation*, 9(2):159–195, 2001. ISSN 0094243X. doi: 10.1063/1.2713540.

Kim, Y., Street, W. N., and Menczer, F. Feature selection in unsupervised learning via evolutionary search. In *Proceedings of the sixth ACM SIGKDD international conference on Knowledge discovery and data mining*, pp. 365–369. ACM, 2000.

Langley, P. Crafting papers on machine learning. In Langley, P. (ed.), *Proceedings of the 17th International Conference on Machine Learning (ICML 2000)*, pp. 1207–1216, Stanford, CA, 2000. Morgan Kaufmann.

M. A., E. Multiple Regression Analysis. *Mathematical Methods for Digital Computers*, 1960.

Mallat, S. and Zhang, Z. Matching pursuits with time-frequency dictionaries. *IEEE Transactions on Signal Processing*, 42(12):33973415, 1993.

Maniezzo, V. Genetic evolution of the topology and weight distribution of neural networks. *IEEE Transactions on neural networks*, 5(1):39–53, 1994.

Matthias Feurer, Jan N. van Rijn, A. K. P. G. N. M. S. R. A. M. J. V. F. H. Openml-python: an extensible python api for openml. *arXiv*, 1911.02490. URL https://arxiv.org/pdf/1911.02490.pdf.

Pati, Y., Rezaiifar, R., and Krishnaprasad, P. Orthogonal matching pursuit: recursive function approximation with applications to wavelet decomposition. *Proceedings of 27th Asilomar Conference on Signals, Systems and Computers*, pp. 40–44, 1993. ISSN 1058-6393. doi: 10.1109/ACSSC.1993.342465. URL http://ieeexplore.ieee.org/document/342465/.

Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg, V., Vanderplas, J., Passos, A., Cournapeau, D., Brucher, M., Perrot, M., and Duchesnay, E. Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research*, 12:2825–2830, 2011.

Sørensen, T., Sørensen, T., Sørensen, T., SORENSEN, T., Sorensen, T., Sorensen, T., and Biering-Sørensen, T. A method of establishing groups of equal amplitude in plant sociology based on similarity of species content and its application to analyses of the vegetation on danish commons. 1948.

Tikhonov, A. N. On the stability of inverse problems. In *Dokl. Akad. Nauk SSSR*, volume 39, pp. 195–198, 1943.

Vafaie, H. and De Jong, K. Genetic algorithms as a tool for feature selection in machine learning. In *Tools with Artificial Intelligence, 1992. TAI'92, Proceedings., Fourth International Conference on*, pp. 200–203. IEEE, 1992.

Vanschoren, J., van Rijn, J. N., Bischl, B., and Torgo, L. Openml: Networked science in machine learning. *SIGKDD Explorations*, 15(2):49–60, 2013. doi: 10.1145/2641190.2641198. URL http://doi.acm.org/10.1145/2641190.2641198.

Zill, D., Wright, W. S., and Cullen, M. R. *Advanced engineering mathematics*. Jones & Bartlett Learning, 2011.