Abstract

The majority of machine learning methods and algorithms give high priority to prediction performance which may not always correspond to the priority of the users. In many cases, practitioners and researchers in different fields, going from engineering to genetics, require interpretability and replicability of the results especially in settings where, for example, not all attributes may be available to them. As a consequence, there is the need to make the outputs of machine learning algorithms more interpretable and to deliver a library of “equivalent” learners (in terms of prediction performance) that users can select based on attribute availability in order to test and/or make use of these learners for predictive/diagnostic purposes. To address these needs, we propose to study a procedure that combines screening and wrapper approaches which, based on a user-specified learning method, greedily explores the attribute space to find a library of sparse learners with consequent low data collection and storage costs. This new method (i) delivers a low-dimensional network of attributes that can be easily interpreted and (ii) increases the potential replicability of results based on the diversity of attribute combinations defining strong learners with equivalent predictive power. We call this algorithm “Sparse Wrapper AlGorithm” (SWAG).

1. Motivation

The purpose of any machine learning algorithm is to deliver precise predictions with respect to a response (or responses) of interest, whether dealing with classification or more general regression problems. Given this common goal, the focus of research has been in developing algorithms and methods that make use of attribute transformation, filtering and selection techniques that allow to best predict the response through often complex non-linear functions and/or heuristic procedures. This is the case of simple classifiers such as Support Vector Machines (SVM) or methods such as neural networks and deep learning (with all their adaptations). As a result of these developments it is possible to train these algorithms to obtain highly accurate testing and validation predictions with consequent important gains in terms of decision-making effectiveness in all domains in which such techniques are employed. Nevertheless, while prediction accuracy remains a paramount goal, there has been an emerging push in different fields to obtain “interpretable” predictions (see e.g. Wang, 2019) in order to better understand phenomena and direct future avenues of research. An important area of machine learning research that (indirectly and partially) addresses this need is that of sparse learning (see e.g. Chandrashekar & Sahin, 2014; Zhang et al., 2015) which, in the context of this work, refers to the use of learners that select and make use only of a reduced number of attributes in a dataset (as opposed to all of them). Indeed, aside from guaranteeing reduced computational complexity for prediction when employing fewer attributes and therefore reducing costs for data collection and storage, sparse learners are effective in addressing the common problem of overfitting by excluding attributes that are possibly not informative and that can increase prediction variability. As a consequence, by selecting and making use of a small set of attributes, sparse learners can also lend themselves to being more easily interpreted and can consequently be used a basis to further investigate certain phenomena (for an overview see Chandrashekar & Sahin, 2014).

However, despite their predictive advantages, all the current sparse learning mechanisms select a single learner (with corresponding unique attributes) and, in high-dimensional settings, nevertheless tend to select many attributes especially in a highly correlated environment (see e.g. Meinshausen & Yu, 2009; Vats & Baraniuk, 2013). These features can have important practical impacts in different settings where interpretability and replicability of the learners is of relevance (see e.g. Marigorta et al., 2018; Quinn et al., 2020).
Indeed, from genomics (e.g. Xiong et al., 2001) to online prediction (e.g. Carmona-Cejudo et al., 2011), there are many tasks that require a degree of flexibility in the use of a multitude of (small) subsets of attributes while preserving high predictive performance. For example, (i) in medical studies machines collect different measurements (attributes) for a specific problem (e.g. Draghici et al., 2006); (ii) for online search algorithms every subject provides different attributes (according to their preferences or willingness to disclose information) to determine suggestions or matches (e.g. Vaughan & Chen, 2015); (iii) in pattern recognition, images are collected at different resolutions and therefore a single learner may not be flexible enough to adapt to different image features (e.g. Wang et al., 2018). In addition, interpretability of phenomena can be greatly enhanced when considering a multitude (library) of sparse learners as highlighted by the multimodel inference and model selection uncertainty literature in areas such as sociology and, especially, ecology (see e.g. Burnham & Anderson, 2004; Anderson & Burnham, 2004; Harrison et al., 2018, for an overview). Moreover, the idea of having a library of learners (and possibly of attributes) was considered, for example, in (Caruana et al., 2004) where libraries are created by forward-selection based on ensemble prediction.

Considering the above discussion, this work aims at creating a library of “strong” and low-dimensional learners which can be selected either (i) individually based on attribute availability or based on whether some attributes are of specific interest within a given domain and/or (ii) jointly to generate a low-dimensional network highlighting the intensity and direction of attribute interaction in order to explain the responses of interest. The method we put forward for this purpose consists in a new greedy version of the algorithm that was proposed for gene selection problems in (Guerrier et al., 2016) and overcomes some of its limitations in terms of dimension reduction. We call this development the “Sparse Wrapper Algorithm” (SWAG for short) whose main goal is to explore the attribute space in an “informed” manner to deliver a library of low-dimensional learners, all with high and comparable predictive power. Hence, given a selected learning method, the output of this approach therefore increases the possibility of replicating results and of making use of specific learners of interest while delivering interpretable connections between attributes for possible future directions of research in different domains.

2. The Sparse Wrapper Algorithm

The SWAG combines screening approaches within a general wrapper method to explore the (low-dimensional) attribute space in an effective manner. In order to find a library (set) of learners that take a small number of attributes as inputs and that have high predictive power, the algorithm proceeds in a forward-step manner. More specifically, it builds and tests learners starting from very few attributes until it includes a maximal number of attributes by increasing the number of attributes at each step. Hence, for each fixed number of attributes, the algorithm tests various (randomly selected) learners and picks those with the best performance in terms of training error. Throughout, the algorithm uses the information coming from the best learners at the previous step to build and test learners in the following step. In the end, it outputs a set of strong low-dimensional learners.

Given the above intuitive description, we now provide a more formal description and, for this reason, we define some basic notation. Let $y \in \mathbb{R}^n$ denote the response and $X \in \mathbb{R}^{n \times p}$ denote an attribute matrix with $n$ instances and $p$ attributes, the latter being indexed by a set $S := \{1, \ldots, p\}$. In addition, a generic learning mechanism is denoted as $L := L(y, X)$ with $l$ denoting a general learner which is built by using (i) the learning mechanism $L$ and (ii) a subset of attributes in $X$. Finally, we let $P(A)$ and $|A|$ denote respectively the power set and cardinality of a set $A$. In the following paragraphs we will proceed to describing the algorithm and introduce meta-parameters whose interpretation and selection will be discussed later in Sec. 2.1.

The first choice to make for the algorithm is to determine the maximum dimension of attributes that the user wants to be input in a learner and we denote this parameter as $p_{\max} < p$. Based on this parameter, the SWAG aims at exploring the space of attributes in order to find sets of learners using $\hat{p}$ attributes ($1 \leq \hat{p} \leq p_{\max}$) with high predictive power. To do so, the algorithm makes use of the step-wise screening procedure described in the following paragraphs.

First Step The first screening step starts by using one distinct attribute at a time to create $p$ learners. Once these learners are built, a set of learners $\mathcal{M}^*$ is now available which is indexed by the ordered index set $\mathcal{I} := \{1, \ldots, p\}$ (i.e. each learner $l \in \mathcal{M}^*$ is indexed by a unique element $i \in \mathcal{I}$). Having chosen a measure of predictive error (e.g. a loss function such as the misclassification rate for classification problems), one can then apply $r$-repeated $k$-fold cross-validation to determine the training error of each learner $l \in \mathcal{M}^*$. We denote the vector containing the cross-validation error as $\epsilon^* \in \mathbb{R}^p$ which is also indexed by the set $\mathcal{I}$ (i.e. each learner $l \in \mathcal{M}^*$ is associated with an element in the training error vector $\epsilon^*$). Given this, it is now possible to select a performance quantile $q_{\alpha}$ where $\alpha \in (0, 1)$ is chosen by the user. This quantile is defined such that the following expression holds true: $\frac{1}{p} \sum_{i=1}^{p} \mathbb{I}\{\epsilon_i^* \leq q_{\alpha}\} = \alpha$, where $\mathbb{I}_A$ is the indicator function that takes the value 1 if $A$ is true and 0 otherwise, while $\epsilon_i^*$ denotes the $i^{th}$ element of the vector $\epsilon^*$. The smaller the value of $\alpha$, the smaller the training errors selected. The procedure then selects all the learners whose...
training error is smaller or equal to $q_\alpha^*$ and includes these in a new learner set $\tilde{M}^*$. The set $\tilde{M}^*$ therefore collects one-dimensional attribute learners with high predictive power and therefore also contains a subset of attributes $S^* \subset S$ that can be assumed to be highly informative with respect to the response of interest $y$. This procedure is described in Algo. 1.

**General Step** Fixing a given attribute dimension $\hat{p}$ such that $2 \leq \hat{p} \leq p_{\text{max}}$, the general screening step builds a maximum number $m$ of *distinct* learners, all included in a learner set $M^{\hat{p}}$, that each take combinations of $\hat{p}$ *distinct* attributes. In order to build the $m$ learners, the general step takes the attribute index set $S^*$ from Algo. 1 and a set of learners $\tilde{M}$ in which each learner is of dimension $\hat{p} - 1$ (i.e. each learner in $\tilde{M}$ takes $\hat{p} - 1$ attributes as an input). We let $s_1 \in S := \{s \in P(S^*) \mid |s| = \hat{p} - 1\}$ denote the attribute indices for a specific learner $l \in \tilde{M}$.

In order to build the $m$ learners, the procedure first verifies whether all possible attribute combinations can be used. Indeed, if we denote $p^* := |S^*|$, then the total number of learners that can be built is $\tilde{m} := \binom{p^*}{\hat{p}}$ and, if $m \geq \tilde{m}$, then the learner set $M^{\hat{p}}$ contains all possible learners. However, if $m < \tilde{m}$, then this step randomly selects a learner $l \in \tilde{M}$ and builds a new learner by using the attributes indexed by $s_1$ and a randomly selected distinct attribute from the attribute index set $S^*/s_1$. This step is repeated until $m$ distinct learners are built and included in the learner set $M^{\hat{p}}$.

Once the candidate learner set $M^{\hat{p}}$ is built, the general step of the algorithm closely follows Algo. 1. More specifically, an $r$-repeated $k$-fold cross-validation error $e^{\hat{p}}$ is built and its performance quantile $q_\alpha^{\hat{p}}$ is computed. The main output of this step is then a new learner set $\tilde{M}^{\hat{p}}$ which includes all learners whose training error in $e^{\hat{p}}$ is smaller or equal to $q_\alpha^{\hat{p}}$ (with both $e^{\hat{p}}$ and $M^{\hat{p}}$ being ordered by the same index set $I^{\hat{p}} := \{1, \ldots, m\}$). This general step is described in Algo. 2.

As per its name, the above described algorithms provide a straightforward manner of selecting a set of predictive learners for a given attribute dimension $\hat{p}$. However, as the attribute dimension increases, the number of possible distinct attribute combinations increases exponentially fast. Therefore, as the attribute dimension grows, there is an increased risk of inefficiently exploring the attribute space if one simply randomly picks $m$ attribute combinations. For this reason, the SWAG performs a greedy procedure which uses the information from Algo. 1 to obtain the set of best attributes $S^*$ which is the easiest to explore completely. The next step of the algorithm then takes the set $S^*$ and the set of best learners $\tilde{M}^*$ as the input $\tilde{M}$ for Algo. 2 for attribute dimension $\hat{p} = 2$. At each of the following steps $\hat{p} > 2$, the algorithm defines $\tilde{M} := M^{\hat{p}-1}$. Therefore, when increasing the attribute dimension, the algorithm only considers attribute combinations based on “informative” learners and attributes from the previous dimension. This procedure is repeated for all attribute dimensions until the maximal dimension $p_{\text{max}}$ is reached. Throughout the procedure, the algorithm saves the strong learner sets (whose training error is below the computed quantile) and training error vectors for each dimension $\hat{p}$. This procedure defines the SWAG which is described in Algo. 3. Once the SWAG is run, there are a series of options that can be considered as discussed in the following paragraphs.

**Post-Processing** The output of the SWAG is a set of learners with high predictive power for each dimension of attribute combinations smaller or equal to $p_{\text{max}}$. The user could choose to directly make use of this set to perform predictions based on different sets of attributes or arrange attributes into networks for interpretation and exploration. However, these sets of learners could undergo an additional screening procedure according to the needs of the user.

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**Algorithm 1 First Screening Algorithm**

**INPUTS:** A response $y \in \mathbb{R}^n$ and attributes $X \in \mathbb{R}^{n \times p}$; An attribute index set $S := \{1, \ldots, p\}$; A learning mechanism $L$; A performance percentile $\alpha \in (0, 1)$; the number of repetitions $r$ and the number of folds $k$ to compute the cross-validation training error.

**OUTPUTS:** $S^*; \tilde{M}^*; M^*; e^*$.

1: Using the mechanism $L$, build $p$ learners by using all attributes in the set $S$
2: Create a learner set $M^*$ (with $|M^*| = p$)
3: Build a an $r$-repeated $k$-fold cross-validation error vector $e^* \in \mathbb{R}^p$ and identify the $\alpha$-quantile $q_\alpha^*$ of this vector
4: Create new learner set $\tilde{M}^*$ with learners whose cross-validation error is smaller or equal to $q_\alpha^*$
5: Create attribute index set $S^*$ with attributes included in the learners in the set $\tilde{M}^*$.
Algorithm 2 General Screening Algorithm

INPUTS: A response \( y \in \mathbb{R}^n \) and attributes \( X \in \mathbb{R}^{n \times p} \); An attribute index set \( S^* \subset \{1, \ldots, p\} \) from Algo. 1: A number of attributes \( \tilde{p} \leq p_{\max} \); A learner set \( \mathcal{M} \); A learning mechanism \( \mathcal{L} \); A maximum number of learners \( m \); A performance percentile \( \alpha \in (0, 1) \); the number of repetitions \( r \) and the number of folds \( k \) to compute the cross-validation training error.

1: Define \( \tilde{n} := (\tilde{p}) \)
2: if \( \tilde{n} \leq m \) then
3:   Using the mechanism \( \mathcal{L} \), build all possible \( \tilde{n} \) learners with \( \tilde{p} \) attribute inputs to create learner set \( \mathcal{M}^\tilde{p} \)
4: else
5:   Using the mechanism \( \mathcal{L} \), build \( m \) learners with \( \tilde{p} \) attribute inputs by extracting \( s_i \) from randomly sampled learners \( l \in \mathcal{M} \) and adding an attribute from \( S^* / s_i \) to create learner set \( \mathcal{M}^\tilde{p} \)
6: end if
7: Build an \( r \)-repeated \( k \)-fold cross-validation error vector \( \epsilon^\tilde{p} \) and identify the \( \alpha \)-quantile \( q^*_\alpha \) of this vector
8: Create new learner set \( \mathcal{M}^\tilde{p} \) with learners whose cross-validation error is smaller or equal to \( q^*_\alpha \)

OUTPUTS: \( \mathcal{M}^\tilde{p} \), \( \tilde{p} \), \( \epsilon^\tilde{p} \).

2.1. Meta-Learning Options

For the application of the SWAG, we assume the user has chosen a learning mechanism \( \mathcal{L} \) for which they would like to obtain more interpretable and replicable learners without losing much predictive power. Based on this, the user has to define the meta-parameters of the algorithm and eventually choose an ensemble approach to aggregate the strong learners that are output.

Meta-Parameters The main user-defined parameters for the SWAG are (i) the maximum attribute dimension \( p_{\max} \); (ii) the maximum number of learners \( m \) to be built within each step, and (iii) the performance percentile \( \alpha \). Ideally, with unlimited computing power, the first two parameters would be as large as possible, i.e. \( p_{\max} = p \) and \( m = \binom{p}{\lfloor \frac{p}{2} \rfloor} \). However, this defeats the purpose of the algorithm and therefore the decision of these parameters must be based mainly on interpretability/replicability requirements as well as available computing power and time. Below are some rules-of-thumb for the choice of these parameters:

- \( p_{\max} \): Fixing the available computing power and the efficiency of the learning mechanism \( \mathcal{L} \), this parameter will depend on the total dimension of the problem \( p \). Indeed, the goal of the SWAG is to find extremely small dimensional learners. Therefore, even with very large \( p \), one could always fix this parameter within a range of 5-20 (or smaller) for interpretability and/or replicability purposes. In addition, if a sparse (embedded) method is computationally efficient to run on the entire dataset, this parameter could be set to the number of selected attributes through this method (given computational constraints). Another criterion, when working with binary classification problems, is to use

Computational Complexity The SWAG algorithm is a computationally intense procedure since it builds at most \( p + m \) \( (p_{\max} - 1) \) learners in total which implies that the order of computation for any learner is multiplied by this factor. In addition, the \( r \)-repeated \( k \)-fold cross-validation will add complexity proportionally to the values of \( r \) and \( k \). Nevertheless, it must be recalled that the learners are built on an extremely small number of attributes (which implies computational efficiency for those mechanisms whose complexity highly depends on the number of attributes) and each fitting and cross-validation can be performed in parallel. A more formal study of the complexity of the SWAG and its possible improvement is left for further research.

Ensemble Learning While the set \( \mathcal{M} \) of strong low-dimensional learners can be used individually to obtain accurate predictions in different settings (where, for example, different attributes are available) or collectively to generate interpretable networks, this set could eventually also be used within an ensemble approach. For example the SWAG learners could be included in Bagging (Breiman, 1996), Boosting (Schapire, 1990) or other model-averaging approaches (see e.g. (Raftery et al., 1997)) in order to possibly obtain more stable and accurate predictions.
the Event Per Variable (EPV) rule presented in (Vittinghoff & McCulloch, 2007) and discussed in (van der Ploeg et al., 2014) (see Sec. 3 for example). In future work, this parameter can be implicitly determined by the algorithm based on the training error quantile (or other metric) thereby defining $p_{\text{max}}$ as the attribute dimension where the training error curve stops decreasing significantly similarly to the scree plot in factor or principal component analysis (see e.g. (Cattell, 1966)).

- $m$: Fixing the available computing power and the efficiency of the learning mechanism $\mathcal{L}$, this parameter will determine the proportion of attribute space that will be explored by the algorithm. We know that it depends on the size of the problem $p$ since we necessarily have $m \geq p$ for the screening step of Algo. 1. In addition, this parameter needs to be chosen considering the performance percentile $\alpha$: if $m$ is small and $\alpha$ is small, then the number of strong learners being selected could be extremely low (possibly zero). In general, we would want a large $m$ (so that $\alpha$ can be small) and, remembering that $p^*$ is the number of attributes released from Algo. 1, a rule-of-thumb is to set $m = \left(\frac{p^*}{\alpha}\right)$ (or close to it) in order to explore the entire (or most of the) subspace of two-dimensional learners generated by $p^*$.

- $\alpha$: as discussed in the previous point, this parameter is related to the maximum number of learners $m$. The larger $\alpha$, the more the attribute space is explored. Ideally, we want to choose a small $\alpha$ since we would want to select strong learners (with extremely low training error) and this is possible if $m$ is large enough. Generally good values for $\alpha$ are 0.01 or 0.05, implying that (roughly) 1% or 5% of the $m$ learners are selected at each step.

### 3. Empirical Results

We study the empirical performance of the SWAG with different learning mechanisms and on different datasets taken from the UCI Machine Learning Repository (see Dua & Graff, 2017), ArrayExpress (see Kolesnikov et al., 2015) and from the GitHub repository [https://github.com/rabriser/datamicroarray](https://github.com/rabriser/datamicroarray). More specifically, the chosen learning mechanisms are: (i) Lasso (logistic) (Friedman et al., 2010); (ii) Linear-Kernel Support Vector Machine (L-SVM) (see e.g. Vapnik, 2013); (iii) Radial-Kernel SVM (R-SVM) (Cortes & Vapnik, 1995); (iv) Random Forest (RF) (Breiman, 2001). To ensure a fair comparison, we run all the analyses with the caret R package (see e.g. Kuhn, 2008, for a review). All the hyper-parameters specific to each learning mechanism are set based on common/default choices and are discussed in the supplementary materials. With regards to the datasets, they are the following: (i) Metta (Gyamfi et al., 2018); (ii) LSVT (Tsanas et al., 2013); (iii) Ahus (Haakensen et al., 2016); (iv) Colon (Alon et al., 1999); (v) Leukemia (Golub et al., 1999). The details regarding these data and the choices for the SWAG meta-learning options are listed in Tab. 1.

The choice of the SWAG meta-learning parameters is made in line with the rules of thumb described earlier and with the intent of reducing overall computational time while ensuring a reasonable exploration of the attribute space. More specifically, we choose $0.01 \leq \alpha \leq 0.05$ as a good compromise between fixing an $\alpha$ as small as possible (in order to select strong learners) and the possibility of exploring a considerable portion of the attribute space (see Sec. 2.1). With $m$ depending on the computing time and power available, we
choose \( m \) (as a linear function of \( p_{\text{max}} \)) in order to at least reasonably explore the subspace of two-dimensional learners for all the learning mechanisms and datasets (further discussed in supplementary material). The choice of \( p_{\text{max}} \) is made guided by the EPV rule discussed in (van der Ploeg et al., 2014). A discussion on the sensitivity of the SWAG results with respect to the choice of these meta-parameters can be found in the supplementary material where it can be seen that the outcome is reasonably stable across different values of these parameters. Finally, we choose to apply 10-repeated 10-fold cross-validation (i.e. \( r = 10 \) and \( k = 10 \)) within the SWAG and choose \( \delta = 0.01 \) for the post-processing based on the previously described median rule. With the

\[
\begin{array}{l|ccccccc}
\text{Data} & n_{\text{train}} & n_{\text{test}} & p & p_{\text{max}} & m & \alpha \\
\hline
\text{MeterA} & 69 & 18 & 666 & 6 & 3984 & 0.05 \\
\text{LSVT} & 100 & 26 & 310 & 6 & 1014 & 0.05 \\
\text{Ahus} & 125 & 31 & 15,739 & 8 & 99080 & 0.01 \\
\text{Colon} & 50 & 12 & 2,000 & 4 & 7996 & 0.03 \\
\text{Leukemia} & 58 & 14 & 7,129 & 4 & 10160 & 0.01 \\
\end{array}
\]

above in mind, we present some summary measures of the set of SWAG learners \( \mathcal{M} \) such as their dimensions and their Jaccard diversity indices in order to understand how interpretable (sparse) and how replicable (diverse) the resulting SWAG networks are (see dataset-specific paragraphs further on). Tab. 2 collects this information for all the datasets where, for each dataset and learning mechanism, we provide the range of dimensions of the SWAG learners \(|s_j|\), the median value for the pairwise Jaccard indices for all learners in \( \mathcal{M} \) \((\text{med}_J)\) as well as their range \((\text{range}_J)\). It can be seen how the SWAG learners have all very low dimensions (also as a result of \( p_{\text{max}} \)) and that at least half of the Jaccard indices for all learning mechanisms and datasets are below or equal to 0.5, indicating that there is a reasonable or high level of diversity in the SWAG learners which is essential for replicability as well as interpretability. However, an important aspect to underline is that, while the goal of the SWAG is to deliver the latter two advantages, it comes at (or extremely low) cost in terms of loss of prediction accuracy. Indeed, Fig. 1 represents the test error (denoted as \( \epsilon_{\text{test}} \)) of the original learning methods (i.e. learning methods applied to all attributes), represented by the red dots, and of the respective SWAG learners, represented by a blue rectangle proportional to the range of test errors (a similar figure is available for the training error \( \epsilon_{\text{train}} \) in the supplementary material). It can be seen how in the majority of cases the SWAG learners have close or comparable (if not sometimes better) prediction accuracy with respect to their original versions, with homogeneous and exact accuracy when using Lasso and R-SVM on the Meter A data for example. Hence, the prediction performance is overall preserved while selecting learners of extremely low-dimension (maximum dimension 8) while the Lasso (the only sparse alternative considered) selects between 10 and 26 attributes.

![Figure 1. SWAG test error range \( \epsilon_{\text{test}} \) (blue rectangles) and original learning method test error (red dots). The blue squares imply that the SWAG learners all have the same test error.](image)

Given the fact that prediction accuracy is generally preserved with the SWAG learners, let us investigate the advantages of the SWAG in terms of its main goal which is interpretability (along with replicability which was observed through the Jaccard index above). To do so we consider building low-dimensional SWAG networks, based on the final selected set of learners, and give a brief overview of their advantages for research and interpretation.

**Ultrasonic Flowmeters** The Meter A data is analyzed in (Gyamfi et al., 2018) and collects measurements on ultrasonic flowmeter diagnostics. Achieving good diagnostics regarding the health of a flowmeter is of extreme importance for condition-based maintenance in many industrial sectors such as the oil and gas industry since incorrect measurement can entail considerable economic and material losses (see e.g. TUV-NEL, 2012). In this data the goal is to classify the health of a meter into two classes: “Healthy” (Class 1) or “Installation effects” (Class 2). Given that the attributes are measurements of physical nature, we decide to consider all first-order interactions which finally delivers a total attribute size of \( p = 666 \) (36 original attributes plus \( \binom{36}{2} = 630 \) interactions).

Using the results from Lasso-based SWAG, we can see how the attributes most frequently included in the selected learners (listed in supplementary material) can be arranged

| Data     | \( n_{\text{train}} \) | \( n_{\text{test}} \) | \( p \) | \( p_{\text{max}} \) | \( m \) | \( \alpha \) |
|----------|------------------------|---------------------|------|---------------------|------|--------|
| MeterA   | 69                     | 18                  | 666  | 6                   | 3984 | 0.05   |
| LSVT     | 100                    | 26                  | 310  | 6                   | 1014 | 0.05   |
| Ahus     | 125                    | 31                  | 15,739 | 8             | 99080 | 0.01  |
| Colon    | 50                     | 12                  | 2,000 | 4                | 7996 | 0.03   |
| Leukemia | 58                     | 14                  | 7,129 | 4                | 10160 | 0.01  |
Table 2. For each learning mechanism (main columns) and each dataset (rows), we have the range of SWAG learner dimensions, the median Jaccard index and the range of the Jaccard indices for the SWAG learners.

| Learner   | Lasso          | L-SVM          | R-SVM          | RF          |
|-----------|----------------|----------------|----------------|-------------|
|           | $|s_l|$ | median $J_{\text{med}}$ | range $J_{\text{range}}$ | $|s_l|$ | median $J_{\text{med}}$ | range $J_{\text{range}}$ | $|s_l|$ | median $J_{\text{med}}$ | range $J_{\text{range}}$ | $|s_l|$ | median $J_{\text{med}}$ | range $J_{\text{range}}$ |
| MeterA    | [4, 6] | 0.38 | [0.09, 0.83] | [2, 6] | 0.16 | [0.00, 0.83] | [4, 6] | 0.20 | [0.09, 0.83] | [4, 6] | 0.33 | [0.09, 0.83] |
| LSVT      | [4, 6] | 0.15 | [0.20, 0.83] | [5, 6] | 0.09 | [0.00, 0.83] | [4, 6] | 0.38 | [0.33, 0.83] | [3, 6] | 0.25 | [0.00, 0.83] |
| Ahus      | [6, 8] | 0.15 | [0.00, 0.88] | [7, 8] | 0.23 | [0.00, 0.88] | [5, 8] | 0.23 | [0.00, 0.75] | [5, 8] | 0.25 | [0.00, 0.75] |
| Colon     | [3, 4] | 0.14 | [0.00, 0.75] | [3, 4] | 0.33 | [0.00, 0.75] | [3, 4] | 0.14 | [0.00, 0.75] | [3, 4] | 0.40 | [0.33, 0.75] |
| Leukemia  | [2, 3] | 0.00 | [0.00, 0.67] | [2, 3] | 0.20 | [0.00, 0.67] | [2, 3] | 0.00 | [0.00, 0.67] | 3 | 0.50 | [0.20, 0.50] |

| Percentage of learners including attributes: |
|---------------------------------------------|
| [100%, 75%] | |
| [75%, 50%]  | |
| [50%, 25%]  | |
| [25%, 0%]   | |

| Link intensity between pairs of attributes: |
|---------------------------------------------|
| 100%, 75% | |
| 75%, 50%  | |
| 50%, 25%  | |
| 25%, 0%   | |

Figure 2. Network of attribute importance and pairwise link-intensity in the set of learners $\hat{M}$ for the Meter A dataset using the Lasso-based SWAG results.

Figure 3. Network of attribute importance and pairwise link-intensity in the set of learners $\hat{M}$ for the LSVT dataset using the Radial-Kernel SVM SWAG results.

LSVT  The voice rehabilitation dataset was analyzed in (Tsanas et al., 2013) in order to assess the effectiveness of a computer program called “Lee Silverman voice treatment (LSVT) Companion” which allows patients with Parkinson’s disease to independently progress through a rehabilitative treatment session. Taking data on 126 samples from 14 patients who followed the latter treatment, 310 dysphonia measures were taken on each of them (plus information on sex and age of the patients) and used to understand if they could correctly predict whether the patients’ voices were “acceptable” or “unacceptable” after this treatment. In their analysis, a robust feature selection was used to select 8 attributes (based on the first eight attributes classified by the feature selection method) and subsequently R-SVM was tested (along with RF) to obtain around 90% accuracy in classifying patients’ progress.

There is also scientific interest in determining the attributes (and combinations thereof) that most contribute to the definition, in this case, of a Parkinson’s speech treatment as being acceptable or not. Also in this case, the SWAG learners (based on the R-SVM) can be arranged into a network in order to allow for interpretation as seen in Fig. 3. Based on the SWAG network, researchers interested in improving speech treatment should focus on attributes 6, 7 and 13 which correspond to the 2nd and 3rd Mel-Frequency Cepstral coefficients and on the entropy with base-4 logarithmic coefficients (as well as the interactions between these three
attributes as highlighted by their frequent presence in the same SWAG learners. More information can be found in the supplementary material.

**AHUS - Breast Cancer** The Ahus breast cancer data is analyzed in (Haakensen et al., 2016) and collects breast tissue specimens from patients over a period of 7 years and are profiled according to invasive carcinomas or normal breast tissue samples. Among others, the interest of this data is to understand how genetic biomarkers interact to explain the presence of breast cancer and, also, how these biomarkers can change their impact according to the attributes with which they interact (see e.g. Miglioli et al., 2020). In this sense, the SWAG network represented in Fig. 4 can allow to visualize and determine the size and direction of impact of the attributes according to the other attributes they are connected to.

![Network of attribute importance and pairwise link-intensity in the set of learners $M$ for the AHUS dataset using the Lasso-based SWAG results.](image)

### Discussion and Broader Impact

A feature that could be interesting to investigate further for the SWAG is its possible capacity of selecting learners with fewer redundant attributes (e.g. correlated attributes) with higher probability. In fact, based on its screening procedure, the SWAG selects learners that improve predictive performance and therefore, at each increasing step, reduces the probability of selecting learners that do not improve their performance by adding redundant attributes. The latter attributes will not add further information than that already provided by the attributes included in the learner sets from the previous steps, implying that the new “redundant” learners will probably not be selected in the screening procedure.

In terms of practical consequences, an immediately noticeable impact is that the SWAG provides a reasonable approach to assess the prediction uncertainty of a given learner and also evaluate the performance of any learner compared to the distribution of its training and/or test errors. Indeed, if one does not require a low-dimensional strong learner, then they can always use the SWAG error distribution to understand whether their chosen learning mechanism appears to be better or at least comparable. In this sense, the SWAG error distribution can provide a “validation metric”, in the direction outlined by (Nadeau & Bengio, 2000), to justify the use of a particular learning mechanism for a given dataset (in the same way a goodness-of-fit measure is used in statistical inference).

However, the main impact of the SWAG in our view lies in its library of strong low-dimensional learners. Indeed the algorithm can integrate the advantages of mechanisms such as Random Forest where the importance of attributes can be retrieved based on the Mean Decrease Impurity (MDI) or the Mean Decrease Accuracy (MDA) of each predictor in the forest (see e.g. Ishwaran, 2007; Louppe et al., 2013). Therefore, even learning mechanisms that are characterized by a “black-box”-type of procedure (as for the R-SVM example) can be made interpretable through the use of the SWAG. Moreover, based on the concept of “synonyms”, the multiplicity of strong learners delivered by the SWAG can allow to adequately respond to predictive needs even in cases where many attributes are not collected or stored. For example, in the fields of natural sciences and medicine not all the responses or measurements may be available and a library of learners that can provide accurate prediction can be used to pick the learner(s) that best suit(s) the available information.

Finally, the nature of the SWAG lends itself to the selection of strong learners based on non-convex loss (cost) functions that are different from those used to optimize the learners themselves. Depending on the “cost” of each learner-based decision, the cross-validation error within the SWAG could be evaluated based on asymmetric (or complex) cost func-
tions and finally select learners that perform best in terms of this metric (see e.g. Ting, 2000). This can have impacts in many sectors, from machine-maintenance to patient treatments, where decision-making can often be characterized by asymmetric costs and the availability of limited or very specific sets of information.

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