Learning with Subset Stacking

Ş. İlker Birbil
Amsterdam Business School, University of Amsterdam, 1018 TV Amsterdam, The Netherlands

Sinan Yıldırım & Kaya Gökalp
Faculty of Engineering and Natural Sciences, Sabancı University, 34956 Istanbul, Turkey

M. Hakan Akyüz
Econometric Institute, Erasmus University Rotterdam, 3000 DR Rotterdam, The Netherlands

Abstract: We propose a new regression algorithm that learns from a set of input-output pairs. Our algorithm is designed for populations where the relation between the input variables and the output variable exhibits a heterogeneous behavior across the predictor space. The algorithm starts with generating subsets that are concentrated around random points in the input space. This is followed by training a local predictor for each subset. Those predictors are then combined in a novel way to yield an overall predictor. We call this algorithm “LEarning with Subset Stacking” or LESS, due to its resemblance to the method of stacking regressors. We compare the testing performance of LESS with the state-of-the-art methods on several datasets. Our comparison shows that LESS is a competitive supervised learning method. Moreover, we observe that LESS is also efficient in terms of computation time and it allows a straightforward parallel implementation.

Keywords: regression, subset selection, stacking, feature generation

1. Introduction

This paper concerns the application of subset sampling and aggregation to achieve effective learners with computational efficiency on large-scale data. The general approach is to partition the dataset into (random) subsets on which local predictors are trained. Then, the prediction of test data is achieved by using an aggregation over the local predictors.

Learning with subsets obtained from a given training set is not new and has been quite popular due to its potential to improve generalization performance. Such an approach is called bagging when multiple predictors are treated the same, and their average is used in the aggregation stage as the overall predictor (Breiman, 1996a). Bagging uses sampling with replacement to construct training datasets of the same size as the original dataset, similar to the bootstrapping technique. To achieve savings from a computational perspective as well as further improvements in generalization performance, bagging has been applied to randomly drawn training subsets; such methods are also known as subsample aggregating, shortly called subagging (Bühlmann and Yu, 2002; Andonova et al., 2002; Evgeniou et al., 2004). Wolpert (1992) and Breiman (1996b) propose, the so-called, stacking as an aggregation method. Stacking optimizes the weights of the individual predictors used at the aggregation level and generally provides better prediction accuracy than a single estimator. More recently, Bühlmann and Meinshausen (2015) offers a maximin aggregation approach, called magging, which inherits properties from bagging and stacking. In particular, magging uses a weighted average of the estimators, where subsamples are constructed similarly to bagging and estimator weights are optimized to solve a different optimization problem than the one for stacking.

Although the bagging, stacking, and magging methods all successfully reduce the mean squared error of unstable training mechanisms via aggregation, they lack local proximity information of the samples with respect to training subsets. In this study, we offer a novel method that integrates the

*Corresponding author. Email: s.i.birbil@uva.nl
above ideas within a learning algorithm by using the proximity information of data points to localized subsets. Since our method works with local subsets of samples and resembles stacking by combining multiple learners in a global learner, we call our method “Learning with Subset Stacking” or, in short, LESS. As LESS learns from the predictions of individual learners on the subsets, it can be considered a meta-learning algorithm.

The following outlines how LESS works. First, (random) subsets are formed that are concentrated around different points in the input space. Once subsets are constructed, a local predictor is trained over each sample subset. Following the local training step, all samples are then transformed into a modified feature space. The modified feature for an input point is a vector of weighted predictions obtained for that training sample by the local predictors. This weighting is carried out in such a way that the local predictions for that input are assigned importance by the distances of their corresponding subsets to the input point. At the global level, an aggregate prediction is performed on the transformed feature space and the responses. As can be deduced from this description, LESS is very generic and can be applied to most regression problems. The ultimate prediction model depends on the local learners, the distance-based scaling function, and the global learner. See Figure 1 for a schematic view of LESS.

LESS has similarities with bagging, stacking, and magging, as well as the existing local learning or aggregation methods. Nevertheless, the mechanism for the selection of subsets and the adopted approach for global learning are different from each one of those methods. LESS can also be considered a local learning method. There are several local learning methods in the literature; a non-exhaustive list contains kernel regression (Nadaraya, 1964), the locally estimated scatterplot smoothing (Cleveland, 1979), Bayesian committee machine (Tresp, 2000; Liu et al., 2018), Gaussian process regression (Rasmussen and Williams, 2006), mixture-of-experts methods (Rasmussen and Ghahramani, 2001; Meeds and Osindero, 2005; Shahbaba and Neal, 2009; Peralta and Soto, 2014), and locally linear ensemble for regression (Kang and Kang, 2018). LESS differs from each one of them in the way it creates the data subsets and combines the local predictions. By constructing a feature vector for each data point from the local predictions, LESS is also related to feature learning methods (Bengio et al., 2013; Le-Khac et al., 2020). Parallelisms can also be made between LESS and Fuzzy Inference Systems (FIS); see e.g., Mamdani (1974); Takagi and Sugeno (1985) for the foundations and Babuska (1998) for a book review, and Shihabudheen and Pillai (2018) as an excellent survey on fuzzy inference systems. Especially, the adaptive neuro-fuzzy generalization of FIS, namely ANFIS (Jang, 1993), has been a popular framework for modeling non-homogenous input-output relations. The relation of ANFIS to LESS is due to the existence of subsets and the way the final output is formed as a combination of the outputs of those subsets, in both models. However, LESS and ANFIS differ on a methodological level, especially in terms of the approach in the design and combination of their subsets. LESS can also be transformed into a Takagi-Sugeno (TS) type model when both local and global learning steps are achieved by linear or convex programs. Nevertheless, LESS brings different perspectives to subset creation, local and global learning as well as interpretability of the results. We discuss LESS in relation to other methods in detail in Section 4.

Our computational study on a set of regression problems has shown that LESS is quite competitive among many well-known learning methods. The experiments have also yielded that LESS is faster than most of the compared methods, and it lends itself to a parallel implementation in a straightforward manner thanks to its use of multiple subsets of the samples.

The paper is organized as follows: In Section 2 we present the proposed learning algorithm, LESS. In Section 3, we show the performance results of LESS in comparison against state-of-the-art methods.
on several different data sets. We elaborate on the relation of LESS with other methods in Section 4. In Section 5, we conclude the paper, mention challenges for LESS, and discuss potential solutions as well as extensions of LESS.

2. LEarning with Subset Stacking

In this section, we first present the methodology behind LESS generically. Then, we give an example of LESS with some specific choices and discuss the effects of changing its hyperparameters. After discussing the impact of weighting on LESS, we introduce two possible modifications and obtain two LESS variants.

2.1 General Framework

Suppose that we have the training dataset \( \{(x_i, y_i) : i = 1, \ldots, n\} \), where \( x_i \in \mathbb{R}^p \), for some \( p \geq 1 \), stands for the input vector, and \( y_i \in \mathbb{R} \) denotes the scalar output value for the data point \( i \in \{1, \ldots, n\} \). To simplify our exposition, we shall denote the dataset by \((X, y)\). Specifically, \( X \) is an \( n \times p \) matrix whose row \( i \) is \( x_i^\top \), and \( y \) is the \( n \times 1 \) vector of outputs \( y_1, \ldots, y_n \).

Figure 1 shows a depiction of LESS. In the subsequent part, we describe the steps of LESS in the following order: subset selection and local learning, feature generation, global training, and averaging.

2.1.1 Subset selection and local learning

The first step of our learning algorithm is to generate a collection of subsets \((X_j, y_j) \subseteq (X, y)\), \( j = 1, \ldots, m \). We do not impose a restriction to partition the dataset into mutually exclusive, collectively exhaustive subsets. Different subsets may have common samples or there may exist a sample that does not belong to any one of the subsets.
The core idea of our approach is to train a different model with the data points in each subset. That is, for a given input point \( x \), we obtain its prediction by training a learning method \textit{locally} with the subset \( (X_j, y_j) \). We denote this local prediction by \( \mathcal{L}(x|X_j, y_j) \).

It is worth noting the requirement for the method that the selected subsets be localized. Localness is necessary for the trained model to capture the input-output relation in the locality of the center of the subset. One way to ensure localness is as follows: First, we randomly select \( m \) input points from \( X \) as anchors, and then for each anchor, we construct a subset by selecting \( k \)-nearest samples to the anchor. Clearly, the performance of this simple method depends on the random location of the subsets \( (X_j, y_j) \), \( j = 1, \ldots, m \). While this method is straightforward to implement, a principled alternative could be using clustering techniques, such as \( k \)-means or spectral clustering. We shall discuss such variants in Section 2.4.

Note that each local model is trained independently of others. Therefore, the local models can be trained in a trivially parallel fashion. Moreover, each local model works with only a subset of data samples, and hence it is faster to train each one of them.

2.1.2 Feature generation One expects that prediction at an input point \( x \) is more reliable when a sample is \textit{closer} to set \( X_j \). Thus, we also define a weighting function \( w_j(x) \) that is inversely related to the distance between the sample \( x \) and the subset \( X_j \). Then, for each input \( x_i \) in the dataset, we generate a \textit{feature vector} of weighted predictions:

\[
z(x_i) = [w_1(x_i)\mathcal{L}(x_i|X_1, y_1), \ldots, w_m(x_i)\mathcal{L}(x_i|X_m, y_m)]^\top.
\]

To simplify our notation in the subsequent part, we will refer to \( z(x_i) \) as vector \( z_i \) with the components \( z_{ij} = w_j(x_i)\mathcal{L}(x_i|X_j, y_j) \) for \( j = 1, \ldots, m \).

The weights \( w_j(x) \) are based on a distance metric \( d(\cdot, \cdot) : \mathbb{R}^p \times \mathbb{R}^p \rightarrow [0, \infty) \) such that \( w_j(x) \) is inversely related to the distance \( d(x, \bar{x}_j) \), where we define \( \bar{x}_j \) to be the centroid of subset \( j \). One way to choose the weights, which we also adopt in this work, can be

\[
w_j(x) = \frac{\exp \{-\lambda d(x, \bar{x}_j)\}}{\sum_{j'=1}^{m}\exp \{-\lambda d(x, \bar{x}_{j'})\}}
\]

for some \( \lambda \geq 0 \). We note that \( \bar{x}_j \) can also be any representative point in subset \( X_j \), other than its centroid, that could be used to determine the distance. The parameter \( \lambda \) determines the extent to which the distance factor should be taken into account. If \( \lambda \) is small, the predictor weights are closer to each other; if \( \lambda \) is large, then the closer predictors are given more weights than the farther ones. In Section 2.3 we give a discussion on two extreme choices of \( \lambda \). The parameter \( \lambda \) can be tuned by using the training data, \textit{e.g.}, with cross-validation.

2.1.3 Global learning The next step is to train a \textit{global} learning method that results in a mapping from the generated feature vector \( z_i \) to the output value \( y_i \) for \( i = 1, \ldots, n \). Let \( Z \) be the \( n \times m \) matrix, whose row \( i \) is the feature vector \( z_i^\top \) for input \( i \). The output of this global method, when fed by a feature vector \( z \), can be denoted as \( \mathcal{G}(z|Z, y) \). After \textit{LESS} is trained, the prediction for a test point \( x_0 \in \mathbb{R}^p \) simply becomes

\[
\hat{y}_0 = \mathcal{G}(z_0|Z, y)
\]
with \( z_{0j} = w_j(x_0)\mathcal{L}(x_0|X_j, y_j) \) for \( j = 1, \ldots, m \).

**Remark 2.1 (Relation to kernel methods)** It is worth pointing out the relation between LESS and the kernel approach that is used by many learning methods, such as support vector machines, kernel ridge, and Gaussian process regression. Considering the relation in (1), we can define for any two vectors \( x_s \) and \( x_t \), the kernel as

\[
\kappa(x_s, x_t) = z_s^\top z_t = \sum_{j=1}^{m} w_j(x_s)\mathcal{L}(x_s|X_j, y_j)\mathcal{L}(x_t|X_j, y_j)w_j(x_t).
\]

If the fitted local models are linear regressors, with each \( \mathcal{L}(x|X_j, y_j) = v_j^\top x \) for some \( v_j \in \mathbb{R}^p \), then by using our notation, the kernel simplifies to

\[
\kappa(x_s, x_t) = x_s^\top V(x_s)V(x_t)^\top x_t,
\]

where for any \( x \in \mathbb{R}^p \), the \( p \times m \) matrix \( V(x) \) is defined such that its column \( j \) is simply \( v_jw_j(x) \). The derivation above also shows that if we use a global learning method that works with kernels, then we may not need to store the \( Z \) matrix explicitly.

### 2.1.4 Averaging

When the subsets are chosen randomly, e.g., via sampling anchor points, LESS can also benefit from averaging over repetitions to reduce the variance. Averaging is a typical approach that is applied by ensemble methods. For LESS, this simply corresponds to applying the procedure described above \( r \) times and taking the average. If we denote the replication \( \ell \) with a superscript, then the overall prediction for a test point \( x_0 \in \mathbb{R}^p \) with averaging leads to

\[
\hat{y}_0 = \frac{1}{r} \sum_{\ell=1}^{r} G(z_{0j}^{(\ell)}|Z^{(\ell)}, y),
\]

where \( z_{0j}^{(\ell)} = w_j^{(\ell)}(x_0)\mathcal{L}(x_0|X_j^{(\ell)}, y_j^{(\ell)}) \) for \( j = 1, \ldots, m \).

### 2.2 Linear Models as Local and Global Learners

Let us explain LESS in a simple scenario where the local and global learners are all linear. This setting is also the default LESS we have used in our implementation. We assume that either the data is centered or, equivalently, every \( x_j \) has its first element equal to one for the model to accommodate an intercept parameter. We consider the standard linear regression model for training local models, that is, \( \mathcal{L}(x|X_j, y_j) = v_j^\top x \) for some \( v_j \in \mathbb{R}^p \). For instance, assuming \( X_j \) is full rank\(^\dagger\), the ordinary least squares solution leads to

\[
v_j = (X_j^\top X_j)^{-1}X_j^\top y_j.
\]

Using these parameters, we obtain

\[
z_{ij} = v_j^\top x_i w_j(x_i), \quad i = 1, \ldots, n; \quad j = 1, \ldots, m.
\]

\(^\dagger\)When \( X_j \)'s are rank deficient, possibly because \( p > k \), where \( k \) is the number of rows in \( X_j \), one can use a regularizing parameter \( \eta > 0 \) and obtain \( v_j = (X_j^\top X_j + \eta I)^{-1}X_j^\top y_j \) instead.
For the global learning method $\mathcal{G}(z|Z,y)$, we again apply the standard linear regression model, but this time regress on the feature vector $z$. If we denote the ordinary least squares solution with $\beta = [\beta_1, \ldots, \beta_m]^\top$, then provided $Z$ is full rank, we can write

$$\beta = (Z^\top Z)^{-1} Z^\top y.$$  \hfill (3)

Writing the overall prediction at a test point $x_0$ as

$$\hat{y}_0 = \sum_{j=1}^{m} (v_j^\top x_0)[w_j(x_0)\beta_j],$$  \hfill (4)

we see that the overall prediction is a *locally linear combination* of the local predictions, where the coefficient for the $j$'th predictor is $w_j(x)\beta_j$, which depends both on the proximity of the test point $x_0$ to the training subset $X_j$ and the associated regression coefficient of the $j$'th local model within the global predictor. A related interpretation stems from rewriting the above as

$$\hat{y}_0 = x_0^\top \left[ \sum_{j=1}^{m} v_j w_j(x_0) \beta_j \right],$$  \hfill (5)

which implies that the prediction for a test sample is also a locally linear combination of $x_0$. Here, the coefficients of the linear combination are locally determined, that is, they depend on $x_0$. It is important to note that whenever linear models (e.g., ridge regression, Lasso, elastic net) are used for local and global learners, we obtain sample-dependent weight for each feature as in (5). This immediately lends itself to local explanations for the test samples. Consequently, after training LESS with linear models one does not need to consult local interpretation methods, like the infamous SHAP and its extensions (Lundberg and Lee, 2017).

### 2.2.1 Numerical demonstration

Figure 2 illustrates how LESS works, as described in this example, on a dataset generated by adding noise to a trigonometric function. Blue circles represent the samples used for training and orange circles show the samples in the test set. The black line segments in the figure are the local predictions obtained by fitting the linear regressors for each sample subset $X_j$. These predictions can be seen to follow the general pattern of the dataset. For the global method, we have again applied the standard linear regression model to the transformed data.

![Figure 2: Demonstration of local models in LESS on one-dimensional synthetic dataset.](image)
Figure 3 illustrates how the number of subsets \((m)\) and the number of replications \((r)\) change the behavior of LESS. The original unknown model is the same trigonometric function used in Figure 2. We first train each LESS model using \(n = 200\) randomly generated samples with the specified hyperparameter values for \(m, r,\) and \(k = n/m\). The subsets are constructed by randomly sampling \(m\) anchor points as we discussed in Section 2.1.1. The trained models are used to plot the corresponding subfigures in Figure 3. In each row of the figure, we notice that increasing the number of subsets assists LESS in identifying the nonlinear structure of the unknown model. However, the last column also shows that when the number of subsets is too high, the variance also increases. This can be considered overfitting. We observe the smoothing effect of averaging as the number of replications increases at each column of the figure. For the example problem, the unknown function is closely approximated when the number of subsets and the number of replications are both 20.

![Figure 3](image)

**Figure 3**: The effects of changing the number of replications \((r)\), the number of subsets \((m)\), and the number of neighbors \((k)\). Notice that \(n = m \times k\). The subsets are constructed by randomly selecting \(m\) anchor points.

### 2.3 Effect of Weighting

Recall that the feature vector \(z_i^j\) for the input point \(x_i\) is constructed such that its \(j\)'th element is \(z_{ij} = w_j(x_i)\mathcal{L}(x_i|x_j, y_j)\), where \(w_j(x_i)\) is a distance-based weight for subset \(j\) at the input point \(x_i\). In this section, we investigate the effect of the weighting function on the behavior of LESS. For analysis' sake, we will stick to our default implementation in Section 2.2, where linear regression is used for both the local and the global learning phases. Recall that this leads to

\[\mathcal{L}(x_i|x_j, y_j) = x_i^T v_j \text{ with } v_j = (X_j^T X_j)^{-1} X_j^T y_j.\]

for the local models and to the prediction

\[\hat{y}_0 = \sum_{j=1}^{m} (v_j^T x_0) w_j(x_0) \beta_j \text{ with } \beta = (Z^T Z)^{-1} Z^T y.\]
for the global model. We specifically consider the weighting function in (2), although it will become clear that the subsequent discussion can be applied to many other sensible choices for $w_j(x)$. In (2) we have $w_j(x) \propto \exp\{-\lambda d(x, x_j)\}$ with $\sum_{j=1}^m w_j(x) = 1$ for all $x$. Therefore the hyperparameter $\lambda \geq 0$ controls the amount of impact of the subsets on each other.

We discuss the two extreme cases for this hyperparameter, namely, $\lambda = 0$ and $\lambda \to \infty$. The first extreme case is obtained with $\lambda = 0$, which removes the effect of the distance function.

**Proposition 2.1** Let $V$ be the $p \times m$ matrix whose $j$'th column is $v_j$. If $V$ has rank $p$, then LESS reduces to ordinary least squares (OLS) with $\lambda = 0$.

**Proof.** When $\lambda = 0$, all predictions from the subsets will be weighted equally with $w_j(x) = 1/m$ for all $j = 1, \ldots, m$. Let $V$ be the $p \times m$ matrix whose $j$'th column is $v_j$. Then, with equal weights, we have $z_i = V^T x_i / m$ and $Z = XV / m$. The global model finds a $\beta$ such that $\|Z \beta - y\|_2^2$ is minimized. On the other hand, consider minimizing $\|Xb - y\|_2$ with respect to $b$, and let $b^*$ be a solution. Since $V$ has rank $p$, the column space of $Z$ is spanned by the columns of $X$, and as a result there exists a $\beta$ which minimizes $\|Z \beta - y\|_2^2$ and satisfies $V \beta = b^*$. Therefore, the prediction at $x_0$ is $\beta^T V^T x / m = b^*^T x_0$. This concludes that LESS reduces to OLS.

It is worth emphasizing that it is not necessary for the subsets $(X_j, y_j)$, $j = 1, \ldots, m$ to be disjoint, nor is it for them to cover all data points for the above analysis to hold. The only requirement for the exact recovery of OLS is that the rank of $V$ is $p$.

The second extreme case is obtained with $\lambda \to \infty$, which corresponds to choosing the prediction of the local model whose center is at the minimum distance from the testing point. Our result for this case requires a specific way to choose the subsets, which is typically met by clustering methods.

**Proposition 2.2** Assume each data point $x_i$ belongs to the subset to whose center it is closest. Then, as $\lambda \to \infty$, LESS reduces to a collection of non-interacting local models: If a test point $x_0$ is closest to subset $j$, the prediction by LESS at $x_0$ is given by $v_j^T x_0$.

**Proof.** Given the subsets, let $c_i$ be the number of the subset whose center is closest to the data point $x_i$. Then, as $\lambda \to \infty$, the feature vector $z_i$ has for $j = 1, \ldots, m$, the components

$$z_{ij} = \begin{cases} x_i^T v_j, & \text{for } j = c_i; \\ 0, & \text{otherwise}. \end{cases}$$

This means that the subsets do not learn from each other, and for each $j \in \{1, \ldots, m\}$, (3) reduces to finding the component $\beta_j$ that minimizes

$$\sum_{i:c_i=j} (x_i^T v_j \beta_j - y_i)^2.$$ 

(This is solved at $\beta_j = \sum_{i:c_i=j} y_i / \sum_{i:c_i=j} x_i^T v_j$.) Moreover, due to the assumption in the proposition, subset $j$ contains exactly all of those $x_i$'s with $c_i = j$. Thus, the minimization problem above for $\beta_j$ becomes

$$\min_{\beta_j} \|X_j(X_j^T X_j)^{-1} X_j^T y_j \beta_j - y_j\|_2^2$$
which is solved at $\beta_j = 1$. The leads to the fact that the global model predicts the response at a test point $x_0$ as $v_j^\top x_0$, the prediction of the local model of the closest subset to $x_0$.

The two extreme cases demonstrate the critical role of the distance function in the communication level among the subsets. Therefore, it is natural to take $\lambda$ as a hyperparameter that could be tuned, e.g., by cross-validation.

**Remark 2.2 (Unnormalized weights)** The weights in (2) are normalized so that they sum to one. It is also possible to use unnormalized weights when generating the feature vectors, such as $w_j(x) = \exp\{-\lambda d(x, \bar{x}_j)\}$ following the example of (2). Such a choice may be less intuitive; for example, the above analysis on the effect of $\lambda$ does not hold with unnormalized weights. However, unnormalized weights may be useful when it is desired to have predictions with small magnitudes as the test points are far away from all of the subsets, to reduce the prediction variance.

2.4 LESS Variants

The general framework of LESS allows obtaining different variants by modifying several steps detailed in Section 2.1. Here, we shall discuss two immediate choices: clustering for subset selection, and using a separate validation split of the dataset for global learning.

The first choice is to apply a clustering method in place of subset selection. Some of the clustering methods require setting the number of clusters in advance, like $k$-means, and others, like $X$-means clustering (Pelleg and Moore, 2000), determine the number of clusters automatically. In either case, these clusters constitute the subsets in LESS. Unlike selecting the subsets with anchor points, clustering methods entail obtaining subsets with varying sizes and they partition the dataset into mutually exclusive, collectively exhaustive subsets. Note that if the clustering method is not stochastic, or in other words, it does not produce different clusters by varying random seeds, then the averaging step can safely be omitted.

The second choice is based on splitting the training dataset into two parts. The first part is used for local learning, whereas the second part is reserved for global learning. This can be considered a validation approach since the local predictors and the global predictor are trained with independent parts of the dataset. We expect that this approach may decrease the variance of the resulting LESS variant by reducing the potential to overfit to the same dataset used for both local and global learning. However, there is also a trade-off because splitting the dataset into two parts decreases the sizes of the training datasets. With such smaller training datasets, the performances of the local and global predictors may deteriorate. We shall also conduct numerical experiments with these variants in our next section.

3. Computational Experiments

We have first tested LESS on publicly available datasets with varying sizes ($n \times p$): abalone (4, 176 × 7), airfoil (1, 503 × 5), housing (505 × 13), cadata (20, 640 × 8), ccpp (9, 568 × 4), energy (19, 735 × 26), cpu (8, 192 × 12), superconduct (21, 163 × 81), and msd (515, 345 × 90). These datasets are all from the UCI repository by Dua and Graff (2017) except cadata (Pace and Barry, 1997).

In all our experiments, we have normalized the input as well as the output. Our computational
study is conducted in Python, and our open source implementation is available online\textsuperscript{‡}. All the results of this section can be reproduced using the scripts that we have also shared on the same web page. We have mostly used a fixed set of parameters for LESS. We shall refer to this method as default LESS subsequently, and the following definition explicitly states its parameters.

**Definition 3.1** The default LESS uses linear regression for both local and global estimators. The percentage of samples is set to determine the number of neighbors ($k$), and then the number of subsets $m = \lceil n/k \rceil$. The subsets are created by selecting $m$ anchors randomly. For weighting in (2), we use for any $x, x' \in \mathbb{R}^p$ the distance function $d(x, x') = \|x - x'\|_2$ along with $\lambda = m^{-2}$. The number of replications ($r$) is set to 20.

We next present the results of our numerical experiments. With all our experiments that require performance measurement and hyperparameter tuning, we have applied $5 \times 4$ nested cross-validation; that is, five-fold cross-validation is used for train-test split, and four-fold cross-validation is used for hyperparameter tuning. The mean-squared error (MSE) results are reported after averaging over five test splits.

### 3.1 Ablation Study

Our first set of experiments is devoted to showing that both weighting and global learning play crucial roles in the success of LESS. This leads to our ablation study results reported in Figure 4. To this end, we have used the default LESS as in Definition 3.1 and stripped it off either the weighting part (NoW-G), the global learning part (W-NoG), or both (NoW-NoG) to obtain different methods. More concretely, NoW-G corresponds to constructing the feature vector $z_i$ at $x_i$ with the components $z_{ij} = \mathcal{L}(x_i | X_j, y_j), j = 1, \ldots, m$, W-NoG corresponds to predicting the output for a test point $x_0$ with $\hat{y}_0 = \sum_{j=1}^m \mathcal{L}(x_0 | X_j, y_j)w_j(x)$, and NoW-NoG corresponds to predicting the output for a test point $x_0$ with $\hat{y}_0 = \frac{1}{m} \sum_{j=1}^m \mathcal{L}(x_0 | X_j, y_j)$. For each method, we have only tuned the percentage of samples that can be selected from the set $\{1\%, 5\%, 10\%, 20\%\}$.

Figure 4 compares the results of default LESS against the results obtained with the different methods. These results demonstrate that the performance of the bare-bones method (NoW-NoG) improves by adding weighting and global learning. Consequently, default LESS outperforms the other methods in all problems.

### 3.2 Comparison Against Other Methods

To compare the performance of LESS against other regression methods, we have selected 12 well-known approaches. Each method is tuned with the hyperparameter sets given in Table 1 during cross-validation. Linear Regression (LR) does not require hyperparameter tuning. All these methods except, Local Linear Regression (LocR) and Magging (MAG), are available through scikit-learn package (Pedregosa et al., 2011). Like LESS, we have also implemented LocR and MAG using main scikit-learn classes, and our implementations are based on Section 6.3 of Hastie et al. (2009) and the pseudocode\textsuperscript{§} in Bühlmann and Meinshausen (2015), respectively. With the inclusion of Gaussian

\textsuperscript{‡}https://github.com/sibirbil/LESS

\textsuperscript{§}We have realized that occasionally the quadratic programming solver fails to find a solution. In those cases, our implementation assigns equal weights to the estimators.
Figure 4: Results of the ablation study. The vertical axis is obtained by scaling the MSE values with the maximum one among NoW-NoG (no weighting, no global learning), W-NoG (weighting, no global learning), NoW-G (no weighting, global learning), LESS (default).

(*NoW-NoG and W-NoG failed to obtain a reasonable result for problem superconduct, and hence they are set to 1.0 to have a proper scaling of the barplot.)

Process Regression (GPR), we end up comparing LESS against three methods that we have summarized under related approaches in Section 4.

Although LESS is a generic approach that allows various choices for its hyperparameters, we have decided to tune only a few of those, so that we can demonstrate ease-of-use and good performance of LESS. In addition to the parameters of default LESS in Definition 3.1, we have also tried the following alternatives in cross-validation: decision tree regressors for local learning, a random forest for global learning, and $\lambda \in \{0.01, 0.1\}$ for weighting. Like in Definition 3.1, we have used the percentage of training samples to set both the number of neighbors and the number of subsets. To that end, the percentage of samples is selected from the set $\{1\%, 5\%, 10\%, 20\%\}$.

The results in Table 2 show that LESS ranks the best in six out of eight problems among all methods in terms of mean squared error values. GB outperforms the other methods in two problems. This performance is followed by MLP, which obtains the least average error for one problem.
Table 1: Hyperparameter sets used for other methods. The default values are underlined.

| Method                          | Hyperparameter Sets                                                                 |
|---------------------------------|--------------------------------------------------------------------------------------|
| Random Forest (RF)              | number of estimators, \{100, 200\}                                                  |
| Adaboost Regressor (ADA)        | number of estimators, \{50, 100\}                                                   |
| Gradient Boosting (GB)          | learning rate, \{0.01, 0.1, 0.5\}; number of estimators, \{100, 200\}               |
| k-Nearest Neighbor (KNN)        | number of neighbors, \{3, 5, 10, 20, 50, 100\}                                       |
| Decision Tree (DT)              | minimum number of samples required to split, \{2, 4\}                               |
| Support Vector Regression (SVR) | regularization parameter, \{0.1, 1.0, 10.0, 100.0\}                                |
| Multi-layer Perceptron\* (MLP)  | learning rate, \{0.0001, 0.001, 0.01\}                                              |
| Local Linear Regression (LocR)  | percentage of samples, \{1\%, 5\%, 10\%, 20\%, 30\%\}                             |
| Kernel Regression (KR)          | kernel, \{poly, rbf\}                                                               |
| Gaussian Process Regression (GPR)| constant for the kernel matrix, \{0.1, 0.0001, 0.000001\}                          |
| Magging (MAG)                   | percentage of samples, \{10\%, 20\%, 30\%\}                                        |

\*maximum number of iterations is set to 10,000 to ensure convergence
Table 2: Computational results obtained with $5 \times 4$ nested cross-validation. The size of each problem is given in parentheses (samples $\times$ attributes). The values show the mean squared error values after averaging over five folds along with the corresponding standard deviations. The smallest average error for each problem is marked with **boldface font**.

| Problem    | LESS | RF  | ADA | GB  | KNN | DT  | SVR | MLP | LR  | LocR | MAG | KR  | GPR |
|------------|------|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|
| abalone    | Avg  | 0.4287 | 0.4618 | 0.7963 | 0.4561 | 0.4693 | 0.9129 | 0.4457 | **0.4223** | 0.4818 | 0.4296 | 0.6618 | 0.4301 | 0.4537 |
|            | Std. | 0.0315 | 0.0338 | 0.0383 | 0.0328 | 0.0389 | 0.0717 | 0.0422 | 0.0331 | 0.0398 | 0.0267 | 0.1294 | 0.0364 | 0.0423 |
| airfoil    | Avg  | 0.0720 | 0.0804 | 0.2962 | 0.0827 | 0.1683 | 0.1481 | 0.1346 | 0.2236 | 0.4900 | 0.1660 | 0.7120 | 0.2380 | 0.1355 |
|            | Std. | 0.0066 | 0.0112 | 0.0202 | 0.0186 | 0.0150 | 0.0316 | 0.0195 | 0.0152 | 0.0501 | 0.0357 | 0.1121 | 0.0166 | 0.0146 |
| housing    | Avg  | 0.1827 | 0.1959 | 0.2063 | **0.1227** | 0.2653 | 0.2076 | 0.1408 | 0.1656 | 0.2900 | 0.1408 | 1.4017 | 0.1427 | 0.2976 |
|            | Std. | 0.0637 | 0.1028 | 0.1211 | 0.0638 | 0.0788 | 0.1095 | 0.0649 | 0.0743 | 0.0525 | 0.0649 | 1.1115 | 0.0681 | 0.0944 |
| cadata     | Avg  | 0.1695 | 0.1821 | 0.7027 | 0.1821 | 0.3566 | 0.2242 | 0.2210 | 0.3639 | 0.2278 | 0.4618 | 0.2418 | 0.2156 |
|            | Std. | 0.0073 | 0.0059 | 0.0465 | 0.0066 | 0.0087 | 0.0089 | 0.0070 | 0.0084 | 0.0132 | 0.0098 | 0.0540 | 0.0065 | 0.0068 |
| ccpp       | Avg  | 0.0365 | 0.0395 | 0.1072 | 0.0374 | 0.0499 | 0.0674 | 0.0533 | 0.0578 | 0.0714 | 0.0467 | 0.0858 | 0.0561 | 0.0521 |
|            | Std. | 0.0025 | 0.0030 | 0.0070 | 0.0033 | 0.0025 | 0.0042 | 0.0025 | 0.0034 | 0.0035 | 0.0027 | 0.0113 | 0.0028 | 0.0024 |
| energy     | Avg  | 1.0002 | 1.1839 | 1.0004 | **1.0002** | 1.0094 | 1.9770 | 1.0097 | 1.0656 | 1.0009 | 1.0193 | 1.0086 | 1.0200 | 1.3223 |
|            | Std. | 0.0079 | 0.0160 | 0.0079 | 0.0081 | 0.0085 | 0.0177 | 0.0074 | 0.0227 | 0.0077 | 0.0074 | 0.0077 | 0.0078 | 0.0334 |
| cpu        | Avg  | 0.0219 | 0.0232 | 0.0726 | 0.0227 | 0.0402 | 0.0504 | 0.0362 | 0.0253 | 0.2888 | 0.0239 | 0.5929 | 0.0571 | 0.2167 |
|            | Std. | 0.0014 | 0.0032 | 0.0076 | 0.0015 | 0.0066 | 0.0071 | 0.0073 | 0.0015 | 0.0446 | 0.0011 | 0.1338 | 0.0175 | 0.0243 |
| superconduct | Avg | 0.0759 | 0.0762 | 0.3042 | 0.0968 | 0.0934 | 0.1189 | 0.1225 | 0.1361 | 0.2500 | 0.1185 | 0.6107 | 0.1560 | 0.1500 |
|            | Std. | 0.0025 | 0.0030 | 0.0161 | 0.0031 | 0.0022 | 0.0031 | 0.0049 | 0.0088 | 0.0055 | 0.0076 | 0.0949 | 0.0041 | 0.0056 |
| Avg. ranking | 1.7500 | 4.7500 | 10.2500 | 3.000 | 7.1250 | 9.3750 | 5.5000 | 6.5000 | 10.2500 | 5.1250 | 11.5000 | 7.7500 | 8.1250 |

Table 3: Confidence intervals regarding the comparison of LESS to the other methods. Upper half: Two-way ANOVA results; Lower half: Friedman's ranking-based results.
We complement Table 2 with statistical many-to-one comparisons between LESS and the other methods. Table 3 shows the two-way ANOVA results using observations $\text{MSE}(i,j,k)$, the MSE for dataset $i$, method $j$, and repetition $k$, based on the assumption $\text{MSE}(i,j,k) = a_i + b_j + e_{i,j,k}$ with $e_{i,j,k} \overset{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2)$ for $i = 1, \ldots, 8; j = 1, \ldots, 13; k = 1, \ldots, 5$. Letting LESS be method 1, we provide the 95% simultaneous confidence intervals for the differences $b_j - b_1$ in Table 3. The $p$-values below the confidence intervals correspond to the hypotheses that LESS and the compared method have the same performance in terms of (expected) MSE. The reported $p$-values and the confidence intervals suggest a significant superiority of LESS over the compared methods, except for GB.

We have also conducted Friedman’s non-parametric test to compare all the methods to LESS, as suggested in Demšar (2006). Friedman’s test is based on the rankings of the methods in terms of the average MSEs given in Table 2. Let $R_{i,j}$ be the ranking of the $j$'th method when it is applied to the $i$'th dataset. The averages $\frac{1}{8} \sum_{j=1}^{13} R_{i,j}$ for each method $j$ are reported in the last line of Table 2. It can be observed that LESS has the lowest overall ranking. Along with those averages, we also report the $p$-values on the last line of Table 3, where each $p$-value corresponds to the null hypotheses that LESS and the compared method have the same (expected) ranking. Friedman’s test is known to be generally less powerful than the two-way ANOVA. This is also the case for our experiments as can be seen from the $p$-values in Table 3. Still, the $p$-values are arguably sufficiently small except for GB and RF, hence the test results largely support the findings of the two-way ANOVA related to the significance of the superiority of LESS.

### 3.3 Computation Times

Figure 5 shows the computation times in seconds obtained with the default LESS for two datasets on a personal computer running macOS 12.0 with Apple M1 Chip equipped with 16GB memory and eight cores. The scatter plots depict that the computation times decrease as the percentage of samples increases, and consequently, the number of subsets decreases. The bar plots show the computation times (in logarithmic scale) of other methods with the same datasets. Except for MLP and KR, we have used the default values suggested by the package maintainers. In MLP we set the maximum number of iterations to 5,000 to ensure convergence, and in KR we have selected the radial-basis kernel as the linear kernel performed very poorly in our experiments. The dashed horizontal line is the computation time of LESS obtained with the value of 5% for the percentage of samples since it is also the default value in our Python implementation. Figure 5 demonstrates that LESS is faster than all other methods except DT and LR, and it is on par with ADA.
Figure 5: (Left) Computation times of LESS in seconds. (Right) Time comparison against other methods. The horizontal dashed line shows the computation time of LESS with its default value of 5% of the samples used for setting the number of subsets to 20.

The local learning phase of LESS can be trivially parallelized. To measure the effect of this straightforward parallel implementation, we have first tried the problem superconduct, which has the largest size among all datasets used in our initial benchmarking. We have also used a much larger dataset from the UCI repository about the year prediction of songs (Dua and Graff, 2017). We refer to this problem as msd, which has 515,345 samples and 90 attributes. These experiments are performed on a server running on 64-bit CentOS 6.5 equipped with 512GB RAM and four Intel Xeon E7-4870 v2 clocked at 2.30 GHz, each having 15 cores (60 cores in total). Each core has a 32KB L1 and a 256KB L2 cache, and the size of the L3 cache is 30MB. This parallel version of LESS is also available via our
Figure 6 shows the speedup gained by increasing the number of processors. We have obtained a steady increase in computation time up to 3.5-fold and 2.5-fold for problems superconduct and msd, respectively. Finally, we have selected four methods and compared their computation times against the parallel version of LESS on problem msd. The remaining methods are omitted because either they do not have an immediate parallel implementation, or they fail to train this large dataset in a reasonable time to include in the comparison. Figure 7 shows that the parallel version of LESS reduces the computation time significantly, and ranks LESS as the second fastest method after LR. RF also benefits from parallelization, and with DT, they are slightly slower than LESS in terms of computation times.

Figure 6: Parallelization performance of default LESS for problems superconduct (21,163 samples, 81 attributes) and msd (515,345 samples, 90 attributes). The plot on the left is obtained with the value of 5% of samples (20 subsets), and the one on the right is obtained with 1% of samples (100 subsets).

Figure 7: Comparison of parallel computation times on problem msd (515,345×90) with 32 threads. The horizontal dashed line shows the computation time of default LESS with 5% of samples (20 subsets).
3.4 Performances of LESS Variants

We have conducted our last experiments on variants of LESS described in Section 2.4. As for subset selection, we have used the $k$-means clustering method. To test the validation approach, we use a 70%-30% split of the dataset for training the local predictors and the global predictor, respectively. Consequently, we obtain three variants of default LESS given in Definition 3.1: LESS-C-V that uses both clustering and validation set, LESS-C that uses only clustering, and LESS-V that uses only validation set.

As before, we have conducted nested cross-validation for performance measurement and hyperparameter tuning. Except for the number of subsets parameter, we have used the same parameter grids given in Section 3.2. For LESS and LESS-V, we have tried the percentage of samples from the set $\{1\%, 5\%, 10\%, 20\%\}$. To have a fair comparison, we have also selected the number of clusters parameter of the $k$-means method from the set $\{5, 10, 20, 100\}$ for both LESS-C and LESS-C-V. Since the $k$-means method produces different clusters with different random seeds, we have also applied the averaging step.

Figure 8 shows the results obtained with different variants. In all problems, except abalone, the variants using a validation set, LESS-V and LESS-C-V are outperformed by their counterparts LESS and LESS-C, respectively. Although using a different subset for validation could decrease the variance, decreasing the sizes of the training sets for local and global learning worsens the performance. Moreover, the variance may already be reduced with the averaging step, and hence, the gain from the validation set could be negligible. Using a clustering method, on the other hand, does occasionally improve the performance in some problems. For instance, LESS-C performs better than LESS for the problems airfoil, housing, and superconduct. Thus, if we had included a clustering method and a validation variant to our hyperparameter tuning, LESS could have become the best performing method for all eight problems studied in Section 3.2 (see Table 2).

Figure 8: Results of LESS variants. Vertical axis is obtained by scaling the MSE values with the maximum one among LESS-C-V (clustering, validation), LESS-C (clustering, no validation), LESS-V (no clustering, validation), LESS (default)
Figure 9 compares the performance of the default LESS with i) LESS-1DT when DT is used as the local estimator, ii) LESS-gRF when RF is used as the global estimator, and iii) LESS-1DT-gRF when DT and RF are used as local and global estimators, respectively. The performance of LESS can be further improved when nonlinear estimators are used for local and global learning. Indeed, except for the abalone and energy datasets, LESS combined with local DT and global RF estimators yields a better performance than its default. For the majority of the datasets, LESS-gRF (RF as the global estimator), the error is lower than LESS-1DT (DT as the local estimator). Overall, the error of default LESS can be reduced up to a quarter of it when alternative local and global estimators are used.

Figure 9: Results of changing local and global estimators in LESS. Vertical axis is obtained by scaling the MSE values with the maximum one among LESS (default), LESS-1DT (DT as local estimator), LESS-gRF (RF as global estimator), LESS-1DT-gRF (DT as local estimator, RF as global estimator)

4. Related Methods

There are several approaches closely related to LESS in the literature. In this section, we discuss the most important ones among them and their relation to LESS.

Stacking: It is worth relating LESS to the well-known method of stacking (Breiman, 1996b) in the light of equation (4). Stacking also learns a linear combination of individual predictions to have a global prediction. However, different than stacking, LESS involves a distance-based weighting \( w_j(x_0) \), and instead of learning the overall coefficient \( w_j(x_0)\beta_j \) for the \( j \)’th predictor, it learns \( \beta_j \) only. The weight \( w_j(x_0) \) stems from the way LESS forms subsets on which it obtains its local predictors, which is another feature of LESS that makes it different from the stacking methods. In default LESS, the subsets are formed by first selecting a sample at random as an anchor, followed by the selection of the \( k \)-nearest samples to that anchor. With such subsets that are concentrated at different locations, it becomes relevant to address distances from and to a subset. LESS uses those distances to take into account the possible heterogeneity in the model: When we predict at a given point, LESS penalizes the
prediction obtained from a subset by the distance between the point and the centroid of the subset.

We would like to point out the generality offered by LESS compared to stacking. The LESS method described in the example above uses the ordinary least squares method for its global learner $G(z|Z, y)$. However, in general, this global learner may be chosen to be any appropriate learning method.

**Magging:** The magging method proposed by Bühlmann and Meinshausen (2015) was mentioned in Section 1. Magging also respects the heterogeneity in data. Magging proposes to use a convex combination of multiple estimators, found based on subsets of data as its final estimator. The coefficients of the convex combination are those that minimize the norm of the vector of final predictions. Since magging is presented in the context of linear models, this weighted combination can be transformed into a weighted combination of predictions at any point as the final prediction. However, there are differences between magging and LESS. First, in magging, the same linear combination of the subset predictions is used everywhere for prediction. In contrast, in LESS, the subset predictions are first scaled based on the distance between the center of their subsets to the input point, and only then those scaled predictions are transformed with a common linear combination to yield the final estimate. Second, magging uses non-local subsets while LESS uses local subsets to compute the first stage predictions before aggregation. Furthermore, magging is based on the idea that any common effect across all subsets will be retained by the optimum convex combination. LESS is arguably more flexible in the sense that it also accommodates heterogeneity caused by different components of a point being active in different locations in the input space.

**Local learning:** Local learning methods are also closely related to LESS. The LOcally Estimated Scatterplot Smoothing (LOESS) method by Cleveland (1979) fits a weighted regression model around each data point. This is a generalization over kernel regression, also known as the Nadaraya-Watson estimator by Nadaraya (1964). Methods like LOESS, which delay their learning until a query is made to the system, are also called “lazy learning” methods. Our implementation of local linear regression (LocR), used for benchmarking in Section 3.2, is a variant of LOESS.

Another related model is the Gaussian process regression (GPR) model (Rasmussen and Williams, 2006). In GPR, a Gaussian process is used to address the distance among the samples during prediction. A covariance matrix of these distances takes higher values when two samples are close to each other. Then, based on that covariance matrix, the prediction function is enforced to take closer values at points in close vicinity of each other. When the size of the dataset is too large to work out the covariance matrix efficiently, subsampling ideas can be used. It is common to resort to subsets (Rasmussen and Williams, 2006, Chapter 8), either chosen greedily or randomly, such as the subset of regressors, subset of data points, and projected process methods. Among those approximate methods, the Bayesian Committee Machine (Tresp, 2000) and its variants (Liu et al., 2018) are examples of aggregation models that are worth mentioning.

Like LOESS and GPR, LESS also tends to rely on the neighbor samples when it performs prediction. This is done via the weighting functions $w_j(·)$, which reduces the effect of a local learner on a distant sample. However, unlike LOESS and GPR, LESS also allows distant local learners to have a larger effect on the prediction by learning the coefficients $\beta_j$, $j = 1, \ldots, m$, in its global learning phase. There is an exception to the way locality is enforced regarding GPR: The covariance matrix of GPR can be chosen to be based on a trigonometric function of distance, therefore capturing a repeated pattern in the model. However, the periodicity assumption can be restrictive, let alone the tuning challenges.

Scalable and local versions of Gaussian process regressors, namely the infinite mixture of Gaussian
process experts, have been proposed by Rasmussen and Ghahramani (2001); Meeds and Osindero (2005). In this model, each data point is assigned to a cluster. The prior for this assignment is constructed with a Dirichlet process, and hence, the number of clusters is unbounded. A separate Gaussian process governs each cluster. Therefore, the cost of this algorithm is cubic in the number of inputs assigned to the largest cluster (which can be limited by design) as opposed to the cost which is cubic in the number of data points in the entire dataset. The idea of clusters is to explore the locality, and also, to benefit from computational savings. As the assignments are latent, they need to be estimated along with other parameters using Markov Chain Monte Carlo (MCMC) algorithm. The initial idea belongs to Rasmussen and Ghahramani (2001), while Meeds and Osindero (2005) proposed a variant with the property of being a generative model for the inputs. For classification, a Bayesian way of the cluster-and-predict method, also based on Dirichlet processes, is given by Shahbaba and Neal (2009).

Although the infinite mixture of Gaussian process experts has the advantage of allowing any number of clusters, it is more costly compared to LESS, since the MCMC algorithm designed for it needs to sweep over all the points in the dataset in every iteration. The mixture of experts and sparsity approaches are combined by Shazeer et al. (2017), who propose the Sparsely-Gated Mixture-of-Experts Layer as a component of a deep learning network. Here, for an input sample, a small number of experts among many are activated by a gating network. The method, although generic, is applied for language modeling and machine translation where the Mixture-of-Experts is applied between layers of a recurrent neural network.

The locally linear ensemble method for regression (Kang and Kang, 2018) performs an expectation-maximization algorithm to form clusters and train simple linear models for each cluster. Prediction is then performed as a weighted average of the local predictions. While the method is simpler, it is more specific compared to LESS in terms of the range of local models and the way the local models are combined. Moreover, while LESS is non-iterative, the method of Kang and Kang (2018) is iterative and it needs to sweep over all the points in the dataset in every iteration, similar to the Gaussian process experts approach.

**Fuzzy inference:** Fuzzy inference systems (FIS) (Babuska, 1998; Mamdani, 1974; Takagi and Sugeno, 1985) are also related to LESS. In particular, the adaptive neuro-fuzzy generalization of FIS, namely ANFIS (Jang, 1993), is a successful prediction and control tool. ANFIS can adaptively model systems benefiting from fuzzy membership functions based on a priori expert knowledge to process inputs. We refer to the works by Pedrycz and Gomide (2007); Piegat (2013) for further details on fuzzy modeling and its usage for prediction.

ANFIS boils down to Takagi-Sugeno (TS) fuzzy models (Takagi and Sugeno, 1985) when linear models are used in the clusters to predict the output. In that respect, the default LESS, with linear local and global models, has similarities with TS fuzzy models as well Yen et al. (1998). That being said, LESS and ANFIS are essentially different both on a technical level and in terms of the approach in the design and combination of clusters. Below, we outline some of the important differences.

(i) **Optimized parameters and computational load:** One difference between LESS and ANFIS is in the number of parameters to learn. In ANFIS, both parameters of the membership functions (corresponding to the weights in LESS) and the consequent parameters (corresponding to the local model parameters in LESS) are learned during training. The training is an iterative procedure, where a back-propagation step is used to optimize the weights and the least-squares method is used to update the consequent parameters. In contrast, LESS does not optimize its distance-based weights; the weight
functions are fixed. A related difference is in the way the consequent parameters of ANFIS, which correspond to the local model parameters in LESS, are learned. While ANFIS learns its consequent parameters simultaneously for all its clusters, LESS learns them separately for each cluster in isolation from the other clusters. These differences suggest that, while ANFIS performs a finer tuning in training, LESS is a lot easier to train with significantly reduced computational complexity.

(ii) Combining the ‘local’ outputs: In ANFIS, the final output is often a weighted average of the linear outputs obtained from the subsets. LESS is somehow more general in combining those ‘local’ outputs: Once the local models are trained, the final output prediction is fit over a projected space where the original data is transformed using weights $w_j(x)$. The mentioned generality is because this global learner can be a nonlinear regressor, such as a decision tree.

Feature learning: LESS is a two-stage algorithm where the first stage somewhat involves representing input variables as feature vectors of predictors. In that sense, LESS can be related to representation/feature learning methods; see, Bengio et al. (2013); Le-Khac et al. (2020) for comprehensive reviews. There are many methods for representation learning, such as those based on sparse representations (Lee et al., 2006) and neural networks (Hinton and Salakhutdinov, 2006). LESS is especially related to those feature learning methods based on techniques that respect the locality of input, such as those involving $k$-means clustering (Coates and Ng, 2012), vector quantization, locally linear embedding (Roweis and Saul, 2000), local coordinate coding (Yu et al., 2009; Yu and Zhang, 2010), feature clustering (Xu and Lee, 2015). Although those methods are also motivated by dimensionality reduction, their relation to LESS is mostly due to their acknowledgment of the non-homogeneity of input data. Moreover, feature learning methods (Xu and Lee, 2015) are directly motivated by the use of dimensionality reduction for regression. LESS is not necessarily a dimension-reduction method, since the generated feature vectors can be even larger in dimension than the original inputs. A major difference between LESS and the mentioned works is that while the mentioned works are unsupervised, LESS uses both input and output to learn its features. An exception to this is the work of Peralta and Soto (2014), where local feature selection is performed in the clusters of a mixture-of-experts model for classification.

Subspace methods: Another line of related research concerns selecting random subsets of input vector components, also known as feature selection. Boot and Nibbering (2019) present asymptotic properties and upper bounds for random subspace methods using random feature selection and random Gaussian weighting of predictors. The dimension of the feature space is reduced by selecting random features. This approach can be counted as another feature learning approach, which is fundamentally different than LESS where the source of randomness is the random sample subset selection, not feature selection.

5. Conclusion

In this paper, we have proposed LESS, a generic regression method for learning a model which behaves diversely over the input space. LESS uses both subsampling and stacking ideas in a novel way. The method can also be seen as a two-layer meta-learning algorithm, where local learners feed their outputs as feature vectors to a global learner. Our numerical experiments have shown that LESS is quite competitive when compared to the well-known regression methods. Moreover, LESS is one of the fastest methods among the competing methods in terms of computation time. This good performance in time can even be improved with a straightforward parallel implementation. The first version of
LESS is released as an open-source Python package.

There are also some limitations of our work as well as some possible extensions that may resolve some of those limitations. The performance of LESS is very promising based on our numerical experiments yet there is no theoretical guarantee of its superiority. We report results by selecting the subsets randomly. However, it is unclear whether this is the best choice. A deterministic selection of subsets that maximizes the average distance between the subsets may help improve the performance of LESS. Likewise, subset selection can be made via optimization, where the objective would be to obtain the best predictions from the local predictors. These ideas need to be tested.

For large datasets, the global learning step in LESS can be time-consuming, especially under specific choices for the global learner that demand the knowledge of the transformed data matrix explicitly. Methods that scale with the data size could be chosen for the global learner to relieve the computational burden. One class of such methods is subsampling-based gradient methods. Also, it may be possible to avoid having to calculate and keep the transformed data matrix while still being able to carry out the calculations. For example, to calculate the ordinary least squares solution in the global learning phase, one does not need to know the transformed data matrix; instead, one can calculate the required matrix multiplications by sequentially processing its columns.

Although in principle LESS can also be applied to classification, it is not clear how the categorical output values should be represented in the transformed data matrix. To this end, we are currently trying different approaches and testing them on standard data sets.

Acknowledgments

We thank Kamer Kaya from Sabancı University for his help with the parallel implementation of LESS.

References

Andonova, S., Eliseeff, A., Evgeniou, T., and Pontil, M. (2002). A simple algorithm for learning stable machines. In Proceedings of the 15th European Conference on Artificial Intelligence, ECAI'02, pages 513–517, NLD. IOS Press.

Babuška, R. (1998). Fuzzy Modeling for Control. Kluwer Academic Publishers, USA, 1st edition.

Bengio, Y., Courville, A., and Vincent, P. (2013). Representation learning: A review and new perspectives. IEEE Transactions on Pattern Analysis and Machine Intelligence, 35:1798–1828.

Boot, T. and Nibbering, D. (2019). Forecasting using random subspace methods. Journal of Econometrics, 209(2):391–406.

Breiman, L. (1996a). Bagging predictors. Machine Learning, 24(2):123–140.

Breiman, L. (1996b). Stacked regressions. Machine Learning, 24(1):49–64.

Bühlmann, P. and Meinshausen, N. (2015). Magging: maximin aggregation for inhomogeneous large-scale data. Proceedings of the IEEE, 104(1):126–135.
Bühlmann, P. and Yu, B. (2002). Analyzing bagging. *The Annals of Statistics, 30*(4):927 – 961.

Cleveland, W. S. (1979). Robust locally weighted regression and smoothing scatterplots. *Journal of the American Statistical Association, 74*(368):829–836.

Coates, A. and Ng, A. Y. (2012). Learning feature representations with K-Means. In Montavon, G., Orr, G. B., and Müller, K.-R., editors, *Neural Networks: Tricks of the Trade: Second Edition*, pages 561–580. Springer, Berlin, Heidelberg.

Demšar, J. (2006). Statistical comparisons of classifiers over multiple data sets. *Journal of Machine Learning Research, 7*(1):1–30.

Dua, D. and Graff, C. (2017). UCI machine learning repository. [http://archive.ics.uci.edu/ml](http://archive.ics.uci.edu/ml).

Evgeniou, T., Pontil, M., and Elisseeff, A. (2004). Leave one out error, stability, and generalization of voting combinations of classifiers. *Machine Learning, 55*(1):71–97.

Hastie, T., Tibshirani, R., and Friedman, J. (2009). *The Elements of Statistical Learning: Data Mining, Inference and Prediction*. Springer, second edition.

Hinton, G. E. and Salakhutdinov, R. R. (2006). Reducing the dimensionality of data with neural networks. *Science, 313*(5786):504–507.

Jang, J.-S. (1993). Anfis: adaptive-network-based fuzzy inference system. *IEEE transactions on systems, man, and cybernetics, 23*(3):665–685.

Kang, S. and Kang, P. (2018). Locally linear ensemble for regression. *Information Sciences, 432*:199–209.

Le-Khac, P. H., Healy, G., and Smeaton, A. F. (2020). Contrastive representation learning: A framework and review. *IEEE Access, 8*:193907–193934.

Lee, H., Battle, A., Raina, R., and Ng, A. Y. (2006). Efficient sparse coding algorithms. In *Proceedings of the 19th International Conference on Neural Information Processing Systems, NIPS'06*, pages 801–808, Cambridge, MA, USA. MIT Press.

Liu, H., Cai, J., Wang, Y., and Ong, Y.-S. (2018). Generalized robust Bayesian committee machine for large-scale gaussian process regression. In Dy, J. and Krause, A., editors, *Proceedings of Machine Learning Research, volume 80*, pages 3131–3140. International Machine Learning Society (IMLS). International Conference on Machine Learning 2018.

Lundberg, S. M. and Lee, S.-I. (2017). A unified approach to interpreting model predictions. In Guyon, I., Luxburg, U. V., Bengio, S., Wallach, H., Fergus, R., Vishwanathan, S., and Garnett, R., editors, *Advances in Neural Information Processing Systems 30*, pages 4765–4774. Curran Associates, Inc.

Mamdani, E. (1974). Application of fuzzy algorithms for control of simple dynamic plant. *Proceedings of the Institution of Electrical Engineers, 121*:1585–1588(3).
Mees, E. and Osindero, S. (2005). An alternative infinite mixture of gaussian process experts. In Proceedings of the 18th International Conference on Neural Information Processing Systems, NIPS’05, pages 883–890, Cambridge, MA, USA. MIT Press.

Nadaraya, E. A. (1964). On estimating regression. Theory of Probability & Its Applications, 9(1):141–142.

Pace, R. K. and Barry, R. (1997). Sparse spatial autoregressions. Statistics & Probability Letters, 33(3):291–297.

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. (2011). Scikit-learn: Machine learning in Python. Journal of Machine Learning Research, 12:2825–2830.

Pedrycz, W. and Gomide, F. (2007). Fuzzy systems engineering: toward human-centric computing. John Wiley & Sons.

Pelleg, D. and Moore, A. (2000). X-means: Extending k-means with efficient estimation of the number of clusters. In Proceedings of the 17th International Conf. on Machine Learning, pages 727–734. Morgan Kaufmann.

Peralta, B. and Soto, A. (2014). Embedded local feature selection within mixture of experts. Information Sciences, 269:176–187.

Piegat, A. (2013). Fuzzy modeling and control, volume 69. Physica.

Rasmussen, C. E. and Ghahramani, Z. (2001). Infinite mixtures of Gaussian process experts. In Advances in Neural Information Processing Systems, pages 881–888.

Rasmussen, C. E. and Williams, C. K. I. (2006). Gaussian processes for machine learning. Series on Adaptive Computation and Machine Learning. MIT Press.

Roweis, S. T. and Saul, L. K. (2000). Nonlinear dimensionality reduction by locally linear embedding. Science, 290(5500):2323–2326.

Shahbaba, B. and Neal, R. (2009). Nonlinear models using Dirichlet process mixtures. Journal of Machine Learning Research, 10(63):1829–1850.

Shazeer, N., Mirhoseini, A., Maziarz, K., Davis, A., Le, Q. V., Hinton, G. E., and Dean, J. (2017). Outrageously large neural networks: The sparsely-gated mixture-of-experts layer. In International Conference of Learning Representations (poster).

Shihabudheen, K. and Pillai, G. N. (2018). Recent advances in neuro-fuzzy system: A survey. Knowledge-Based Systems, 152:136–162.
Takagi, T. and Sugeno, M. (1985). Fuzzy identification of systems and its applications to modeling and control. IEEE transactions on systems, man, and cybernetics, SMC-15(1):116–132.

Tresp, V. (2000). A Bayesian committee machine. Neural Computation, 12(11):2719–2741.

Wolpert, D. H. (1992). Stacked generalization. Neural Networks, 5(2):241–259.

Xu, R.-F. and Lee, S.-J. (2015). Dimensionality reduction by feature clustering for regression problems. Information Sciences, 299:42–57.

Yen, J., Wang, L., and Gillespie, C. W. (1998). Improving the interpretability of tsk fuzzy models by combining global learning and local learning. IEEE Transactions on fuzzy Systems, 6(4):530–537.

Yu, K. and Zhang, T. (2010). Improved local coordinate coding using local tangents. In Proceedings of the 27th International Conference on International Conference on Machine Learning, ICML’10, pages 1215–1222, Madison, WI, USA. Omnipress.

Yu, K., Zhang, T., and Gong, Y. (2009). Nonlinear learning using local coordinate coding. In Bengio, Y., Schuurmans, D., Lafferty, J., Williams, C., and Culotta, A., editors, Advances in Neural Information Processing Systems, volume 22.