asgl: A Python Package for Penalized Linear and Quantile Regression

Álvaro Méndez Civiea∗† M. Carmen Aguilera-Morillo†‡ Rosa E. Lillo∗†

Abstract

asgl is a Python package that solves penalized linear regression and quantile regression models for simultaneous variable selection and prediction, for both high and low dimensional frameworks. It makes very easy to set up and solve different types of lasso-based penalizations among which the asgl (adaptive sparse group lasso, that gives name to the package) is remarked. This package is built on top of cvxpy, a Python-embedded modeling language for convex optimization problems and makes extensive use of multiprocessing, a Python module for parallel computing that significantly reduces computation times of asgl.

keywords: Regression, Variable-selection, High-dimension, Python.

1 Introduction

In this paper, asgl, an open source Python [van Rossum and Drake, 2009] package for solving penalized linear regression and quantile regression models is introduced. While linear regression is very well known and need no introduction, quantile regression is less known. Quantile regression provides an estimation of the conditional quantile of a response variable as a function of the covariates, it is robust against outliers and can deal with heteroscedastic datasets (as opposed to linear regression). Ever since the seminal work from Koenker and Bassett [1978] it has become more and more used in practical applications thanks to these properties.

∗Department of Statistics, Universidad Carlos III de Madrid.
†uc3m-Santander Big Data Institute.
‡Department of Applied Statistics and Operational Research, and Quality, Universitat Politècnica de València.
Penalized regression is a field under intense research nowadays due to the increasing number of problems where high dimensional data (in which the number of variables $p$ is larger than the number of observations $n$) can be seen. It is not uncommon to find this scenario in problems from fields such as genetics [Simon et al., 2013], finances [Rapach et al., 2013] or pattern recognition [Wright et al., 2010] among many others. One of the best known automatic prediction and variable selection alternatives for high dimensional data is lasso (least absolute shrinkage and selection operator) [Tibshirani, 1996], that makes use of an $\ell_1$ norm to provide sparse estimations of the coefficients of the model. After Yuan and Lin [2006] proposed the group lasso penalization, a considerable literature was generated about the selection of variables both at group and within-group levels, among which the sparse group lasso, proposed by Friedman et al. [2010] is worth to remark. This penalization generalizes lasso and group lasso providing solutions that are both between and within group sparse.

The penalizations mentioned above achieve good prediction results, but face the same underlying theoretical problem. They all provide biased solutions due to the usage of constant penalization rates, fact that can affect the quality of variable selection and prediction accuracy. This problem was addressed by Zou [2006] who proposed using what is known as the adaptive idea, that consists on adding some weights previously defined by the researcher to the penalization term. Traditionally, these weights are computed based on non penalized models, fact that limited the usage of adaptive formulations to low dimensional frameworks where non penalized models could be solved. However, Mendez-Civieta et al. [2020] defined an asgl (adaptive sparse group lasso) estimator and proposed a series of weight calculation alternatives based on dimensionality reduction techniques pca (principal component analysis) and pls (partial least squares), that provide very good results in both high dimensional and low dimensional frameworks.

It is possible to find implementations of many of the penalization alternatives discussed above in different programming languages. One can find lasso, group lasso and sparse group lasso penalized linear regression models in R (for example, using the sgl package), lasso and group lasso linear models in Python (in sklearn and group-lasso respectively) and lasso models in Matlab. Regarding quantile regression, it is possible to find lasso penalized models in the quantreg package for R, but no quantile regression penalization alternatives are available in Python or Matlab. Additionally, to the best of our knowledge, there is no statistical software currently implementing the usage of adaptive penalizations, which are known to provide much better results than the non-adaptive counterparts. An overview of this situation is shown in Table 1.

The asgl package solves this problem. It provides an easy to use framework where lasso, group lasso, sparse group lasso, and adaptive versions of all these penalizations can be solved
for both linear models and quantile regression models. It also implements the main weight calculation alternatives proposed in Mendez-Civieta et al. [2020] for adaptive formulations as well as a grid-search based system for optimizing the parameter values using cross validation.

The rest of the paper is organized as follows. In Section 2 the linear regression and quantile regression models are specified, along with lasso, group lasso, sparse group lasso, and adaptive penalizations. In Section 3 the main asgl classes are described in detail. Section 4 then illustrates the usage of this package to a variety of examples. Section 6 concludes.

\section{Theoretical background}

Given a sample of \( n \) observations structured as \( \mathbb{D} = (y_i, x_i), \ i = 1, \ldots, n \) from some unknown population, define a linear model,

\[ y_i = x_i^T \beta + \varepsilon_i, \ i = 1, \ldots, n, \tag{1} \]

where \( y_i \) is the \( i \)-th observation of the response variable, \( x_i \equiv (x_{i1}, \ldots, x_{ip}) \) is the vector of \( p \) covariates for observation \( i \) and \( \varepsilon_i \) is the error term.

\subsection{Least squares and quantile regression}

\subsubsection{Least squares regression}

Least squares regression, usually known simply as linear regression, provides an estimation of the conditional mean of the response variable as a function of the covariates. The solution of this type of models is obtained by minimizing the risk function,

\[ R(\beta) = \frac{1}{n} \sum_{i=1}^{n} (y_i - x_i^T \beta)^2. \tag{2} \]
2.1.2 Quantile regression

Quantile regression, initially proposed by Koenker and Bassett [1978], provides an estimation of the conditional quantile of the response variable as a function of the covariates. Opposed to least squares regression, quantile regression offers robust estimators when dealing with heteroscedasticity and outliers, a fact that has made it increasingly popular in recent years. For a full review on quantile regression we recommend Koenker [2005]. The solution of quantile regression models is obtained from the minimization of the risk function,

$$ R(\beta) = \frac{1}{n} \sum_{i=1}^{n} \rho_{\tau}(y_i - x_i^t \beta), $$

where $\rho_{\tau}(u)$ is the loss function defined as $\rho_{\tau}(u) = u(\tau - I(u < 0))$.

2.2 Penalized regression

We call high dimensional to a framework in which the number of covariates $p$ is larger than the number of observations $n$ ($n < p$). This situation is becoming more and more common, and can be found in problems from different fields such as genetics (Yahya Algamal and Hisyam Lee [2019]), finance (Rapach et al. [2013]) or climate data (Chatterjee et al. [2011]) among others.

2.2.1 Lasso

Regression models including a penalization constraint have become very popular in high dimensional problems, and one of the best known penalization alternatives is lasso. Lasso, initially proposed by Tibshirani [1996], solves the problem,

$$ \hat{\beta} = \operatorname{arg\,min}_{\beta \in \mathbb{R}^p} \{ R(\beta) + \lambda \|eta\|_1 \}, $$

where $R(\beta)$ can be either the linear regression or the quantile regression risk function defined in equations 2 and 3 respectively, and $\lambda$ is a parameter controlling the weight given to the penalization. Lasso sends part of the beta coefficients to zero, yielding solutions that are sparse and performing automatic prediction and variable selection.

2.2.2 Group lasso

There are situations in which data has a natural grouped structure, and group sparsity rather than individual sparsity is desired. One can think, for example, in groups of genetical pathways in the field of genetics, or groups of technical indicators in finances. The problem
of selecting the most important groups, rather than the most important variables was faced by Yuan and Lin [2006] who proposed the usage of a group lasso estimator,

$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^p} \left\{ R(\beta) + \lambda \sum_{l=1}^{K} \sqrt{p_l} \| \beta^l \|_2 \right\},$$

where $K$ is the number of groups, $\beta^l \in \mathbb{R}^{p_l}$ are vectors of components of $\beta$ from the $l$-th group, and $p_l$ is the size of the $l$-th group. Group lasso works in a similar way to lasso, but while lasso provides individual sparse solutions, group lasso provides group sparse solutions, selecting or sending to zero whole groups of variables.

### 2.2.3 Sparse group lasso

Sparse group lasso, initially proposed by Friedman et al. [2010], is defined as a linear combination between lasso and group lasso that generalizes both penalizations providing solutions that are between and within group sparse. This penalization solves the problem,

$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^p} \left\{ R(\beta) + \alpha \lambda \| \beta \|_1 + (1 - \alpha) \lambda \sum_{l=1}^{K} \sqrt{p_l} \| \beta^l \|_2 \right\},$$

where $\alpha$ controls the balance between lasso and group lasso.

### 2.2.4 Adaptive penalizations

All the penalizations defined above face the same problem: they apply a constant penalization rate that provide biased estimates, fact that can affect the quality of the variable selection increasing prediction error. As a solution to this problem, Zou [2006] proposed using what is now known as the adaptive idea, and defined an adaptive lasso. This idea consists of adding some weights previously defined by the researcher to the penalization. Using the adaptive idea, Mendez-Civieta et al. [2020] defined the adaptive sparse group lasso as,

$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^p} \left\{ R(\beta) + \alpha \lambda \sum_{j=1}^{P} \tilde{w}_j |\beta_j| + (1 - \alpha) \lambda \sum_{l=1}^{K} \sqrt{p_l} \tilde{v}_l \| \beta^l \|_2 \right\},$$

where $\tilde{w} \in \mathbb{R}^P$ and $\tilde{v} \in \mathbb{R}^K$ are known weights vectors. Intuitively, if a variable (or group of variables) is important, it should have a small weight, and this way would be lightly penalized. On the other hand, if it is not important, by setting a large weight it is heavily penalized. The adaptive idea enhances model flexibility, improving variable selection and prediction. Observe that adaptive lasso and adaptive group lasso can be defined just in the same way by adding weights to lasso and group lasso respectively.
Figure 1: Contour lines for lasso, group lasso and sparse group lasso penalties in the case of a single 2-dimensional group

2.3 Weight calculation

The usage of adaptive penalizations opens the door to a question on how to estimate the adaptive weights $\tilde{w} \in \mathbb{R}^p$ and $\tilde{v} \in \mathbb{R}^K$. These weights need to be specified by the researcher prior of solving the optimization problem, and in low dimensional frameworks (where $n > p$), they can be computed as,

$$\tilde{w}_i = \frac{1}{|\tilde{\beta}_i|^\gamma},$$

where $\tilde{w}_i$ and $\tilde{\beta}_i$ correspond to the $i$-th element of vectors $\tilde{w}$ and $\tilde{\beta}$ respectively and $\tilde{\beta}$ is the solution vector obtained from the unpenalized (linear or quantile) regression model, $|\cdot|$ denotes the absolute value function and $\gamma$ is a non negative constant. A small $\beta$ coefficient results into a large weight, which is heavily penalized and more likely left outside the final model. On the opposite hand, large $\beta$ coefficients result into small weights that are likely to remain in the final model. However, when dealing with a high dimensional framework solving an unpenalized model is not feasible, rendering impossible the usage of adaptive formulations. As a solution to this problem, [Mendez-Civieta et al. 2020] proposed a series of weight calculation alternatives based on dimensionality reduction techniques pca (principal component analysis) and pls (partial least squares).
2.3.1 pca based on a subset of components

Given the covariates matrix \( X \in \mathbb{R}^{n \times p} \) with maximum rank \( r = \min\{n, p\} \), the matrix of pca loadings \( Q \in \mathbb{R}^{p \times r} \) and the matrix of pca scores \( Z = XQ \in \mathbb{R}^{n \times r} \), this proposal takes advantage of the fact that the pca scores define a low dimensional framework. Consider the submatrix \( Q_d = [q_1, \ldots, q_d]^t \) where \( q_i \in \mathbb{R}^p \) is the \( i\)-th column of the matrix \( Q \), and \( d \in \{1, \ldots, r\} \) is the number of components chosen in order to explain up to a certain percentage of variability, which is fixed by the researcher. Obtain \( Z_d = XQ_d \in \mathbb{R}^{n \times d} \) the projection of \( X \) into the subspace generated by \( Q_d \) and solve the unpenalized model,

\[
\hat{\beta} = \arg \min_{\beta \in \mathbb{R}^d} \left\{ \frac{1}{n} \sum_{i=1}^{n} \rho_r(y_i - z_i^t \beta) \right\}. \tag{9}
\]

Using this solution, it is possible to obtain an estimation of the high dimensional scenario solution, \( \hat{\beta} = Q_d\hat{\beta} \in \mathbb{R}^p \) and compute the weights as,

\[
\hat{w}_j = \frac{1}{|\hat{\beta}_j|^\gamma_1} \quad \text{and} \quad \hat{v}_l = \frac{1}{\|\hat{\beta}_l\|_2^\gamma_2}, \tag{10}
\]

where \( \hat{\beta}_j \) is the \( j\)-th component from \( \hat{\beta} \), \( \hat{\beta}_l \) is the vector of components of \( \beta \) from the \( l\)-th group, and \( \gamma_1 \) and \( \gamma_2 \) are non negative constants usually taken in \([0, 2]\). An in-depth explanation of this process can be read in the original paper.

2.3.2 pca based on the first component

Each pca score is built as a linear combination of the original variables. This means that another alternative for estimating the weights can be defined as simply using the weights from the first pca loading as weights for the adaptive sparse group lasso model,

\[
\hat{w}_j = \frac{1}{|q_{1j}|^\gamma_1} \quad \text{and} \quad \hat{v}_l = \frac{1}{\|q_{1l}\|_2^\gamma_2}, \tag{11}
\]

where \( q_{1j} \) is the \( j\)-th component from \( q_1 \) and defines the weight associated to the \( j\)-th original variable, \( q_{1l} \) is the vector of components of \( q_1 \) from the \( l\)-th group and \( \gamma_1 \) and \( \gamma_2 \) are non negative constants usually taken in \([0, 2]\).

2.3.3 pls based alternatives

In the same way as for the pca proposal, two alternatives of weight calculation using pls are considered: based on a subset of pls components, and based just on the first pls component. It is worth to remark that due to the way in which the pls components are obtained, this
method cannot recover all the original variability from matrix $X$ as opposed to what happens in pca, where this is ensured by the orthogonal loadings.

2.3.4 sparse pca

Sparse pca was initially proposed by [Zou et al., 2006] as a method that computes principal components adding a lasso based penalization to standard pca. This yields to principal components that are sparse linear combinations of the original variables, though are no longer orthogonal. Using the SparsePCA from sklearn package, the asgl package incorporates a weight calculation alternative based on a subset of sparse pca components.

2.3.5 lasso

In addition to the weight calculation alternatives proposed above, the asgl package implements the usage of a lasso penalized model, that can be directly solved in high dimensional frameworks, as a first step for the calculation of adaptive based formulations.

3 Python implementation

The asgl package is built around four main class objects: ASGL, WEIGHTS, CV and TVT, that will be described in detail along this section.

3.1 ASGL class

The ASGL class is the central part of the package. It includes all the necessary code in order to define and solve penalized regression models. The default parameters from the ASGL class are,

```python
model = asgl.ASGL(model, penalization, intercept=True, tol=1e-5,
lambda1=1, alpha=0.5, tau=0.5, lasso_weights=None,
gl_weights=None, parallel=False, num_cores=None, solver=None,
max_iters=500)
```

where the meaning of the arguments is,

* model: A string specifying the model to be solved. Valid alternatives are:
  - "lm" for solving linear regression models ,
  - "qr" for solving quantile regression models,
• **penalization**: A string specifying the type of penalization to be applied. Valid alternatives are:
  - "lasso" for using a lasso penalization,
  - "gl" for using a group lasso penalization,
  - "sgl" for using an sparse group lasso penalization,
  - "alasso" for using an adaptive sparse group lasso penalization,
  - "agl" for using an adaptive group lasso penalization,
  - "asgl" for using an adaptive sparse group lasso penalization,
  - "asgl_lasso" for using an sparse group lasso with adaptive weights in the lasso part,
  - "asgl_gl" for using an sparse group lasso with adaptive weights in the group lasso part,

• **intercept**: Boolean indicating True if the intercept should be fitted or False otherwise,

• **tol**: A floating point number, tolerance for a coefficient in the model to be considered as 0,

• **lambda1**: A number, Python list of numbers or 1D numpy.array of numbers. Parameter $\lambda$ from the penalization definitions in Section 2.2. It controls the level of shrinkage applied on penalizations. If more than one value is provided, the program solves one model for each possible parameter combination found,

• **alpha**: A floating point number, list of numbers or 1D numpy.array of numbers. Parameter $\alpha$ from the penalization definitions in Section 2.2 used in "sgl", "asgl", "asgl_lasso" and "asgl_gl" penalizations. It must be always bounded between 0 and 1. If more than one number is provided, the program solves one model for each possible parameter combination found,

• **tau**: A floating point number between 0 and 1. Parameter $\tau$ indicating the quantile level in quantile regression models. Value 0.5 solves the median regression. Value 0.25 solves the first quartile regression. If the model is set to "lm", then tau has no effect,

• **lasso_weights**: A list of numbers, 1D numpy.array of numbers, or a list made of list of numbers or 1D numpy.array of numbers. Parameter $w$ from Section 2.3 used only in penalizations including the adaptive lasso weights ("alasso", "asgl" and "asgl_lasso"), it includes the values of the adaptive lasso weights, so each inner list
or **numpy.array** must have length equal to the number of predictors in the dataset. Example: given \( X \in \mathbb{R}^{100 \times 10} \) a predictor matrix with 10 covariates, **lasso_weights** can be equal to a list of length 10, an 1D **numpy.array** of length 10, or it can be a list (of any length) made of lists of length 10. In the latter case, each list will be used in order to fit different adaptive models,

- **gl_weights**: A list of numbers, 1D **numpy.array** of numbers, or a list made of list of numbers or 1D **numpy.array** of numbers. Parameter \( v \) from Section 2.3 used only in penalizations including the adaptive group lasso weights ("agl", "asgl" and "asgl_gl"), it includes the values of the adaptive group lasso weights, so each inner list or **numpy.array** must have length equal to the number of groups in the dataset. Example: given \( X \in \mathbb{R}^{100 \times 10} \) a predictor matrix with 10 covariates divided in three groups, **gl_weights** can be equal to a list of length 3, an 1D **numpy.array** of length 3, or it can be a list (of any length) made of lists of length 3. In the latter case, each list will be used in order to fit different adaptive models,

- **parallel**: Boolean that takes the value **False** if it is required that the solver run sequentially (using only one core) or **True** if it is required to run in parallel (using more than one core),

- **num_cores**: An integer number indicating the number of cores to be used if **parallel** is set to **True**. By default, the program will detect the number of cores in the machine and execute the code in the number of cores minus 1. If **parallel** is **False**, **num_cores** has no effect,

- **solver**: A string indicating the solver to be used by **cvxpy** package. It is recommended to leave this parameter with the default value, as the program will automatically select the best solver among the available options,

- **max_iters**: An integer number indicating the number of iterations to be performed by the **cvxpy** solver. It is recommended to leave this parameter with the default value,

The main methods included in this class object are **fit**, **predict** and **retrieve_parameters_value**.

### 3.1.1 fit function

**fit(x, y, group_index)** is the main function in this class. Once an **ASGL** class object is created, a call to the **fit** function solves the model defined there. The parameters in this function are,
• `x`: A 2-dimensional `numpy.ndarray` matrix of predictors where the rows define the observations in the dataset and the columns define the variables.

• `y`: A 1-dimensional `numpy.ndarray` array. The response vector in the problem to solve.

• `group_index`: A 1-dimensional `numpy.ndarray` array of length equal to the number of variables. An index indicating to which group each variable belongs. Example: `group_index=numpy.array([1,2,2,3])` would mean that there are 4 variables, the first belongs to group 1, second and third belong to group 2 and the fourth to group 3. Observe that this parameter is only required when using group based penalizations "gl", "agl", "sgl", "asgl", "asgl_gl".

As stated in the parameter class ASGL definition, the parameters `lambda1` and `alpha` can be defined as either a single number or as a list or `numpy.ndarray` of values, and `lasso_weights` and `gl_weights` can be defined as lists of values or as lists containing those lists of values. The reason for this is that the `fit` function is programmed in a way that, if lists of values are provided for the parameters, it will solve all the models yielding from all possible combinations of the different values. In other words, it creates a grid of possible parameter value combinations and solves all the models in the proposed grid, computing the $\beta$ coefficients from each case. These results are stored as a list in the `ASGL` class object. Usage example:

```python
>>> import asgl

>>> import numpy as np

>>> from sklearn.datasets import load_boston

>>> boston = load_boston()

>>> x = boston.data

>>> y = boston.target

>>> group_index = np.array([1, 1, 1, 2, 2, 2, 3, 3, 3, 4, 4, 4, 5])

>>> model = asgl.ASGL(model="lm", penalization="sgl",
                   lambda1=[0.001, 0.01, 0.1],
                   alpha=[0.1],
                   lasso_weights=[0.1],
                   gl_weights=[0.1])
```
>>> model.fit(x, y, group_index)

>>> coefficients = model.coef_

>>> len(coefficients)
9

First, the `asgl` package is imported. Then, the `BostonHousing` dataset, a well known regression dataset, is imported from `sklearn` package. This dataset will be used in this and the following examples. The dataset is not known to have a natural grouped structure but observe that here a fake `group_index` is provided for the sake of the example. Finally, an `ASGL` class object is created, and the `fit` function is called, solving a model for each possible combination of parameter values `lambda1` (3 values) and `alpha` (3 values), yielding to 9 solutions. If `parallel=True` these 9 models would be solved in parallel, otherwise, they would be solved sequentially.

### 3.1.2 predict function

`predict(x_new)` function computes predictions based on the coefficients provided after executing the `fit` function. The only parameter in this function is,

- `x_new`: A 2-dimensional `numpy.ndarray` with the number of columns equal to the number of columns in the original matrix `x`. `x_new` is the matrix to be used for computing the predictions.

```python
>>> predictions = model.predict(x_new=x)
```

```python
>>> len(predictions)
9
```

From `model` (the `ASGL` class object created in the example above), the `predict` function is called. In this example, `x_new` is simply taken as the original matrix `x`, although in a real analysis, `x_new` would be the test set, or any new set from which a prediction would be required. `predictions` is a list where each element of the list stores the predictions computed using each possible solution from `coefficients`. 
3.1.3 retrieve parameters value function

The retrieve_parameters_value function returns a Python dictionary storing the value of the parameters associated to a solution index from the array of solutions coefficients. The only parameter in this function is,

- param_index: An integer number no larger than the length of the model.coef_list.

```python
>>> model.retrieve_parameters_value(5)
{'lambda1': 0.01, 'alpha': 0.7, 'lasso_weights': None, 'gl_weights': None}
```

This Python dictionary is formed by 4 elements, one for each possible parameter in the model. If the model solved did not use any of the parameters, the function will retrieve the value None for such parameter. For example, in this case an sparse group lasso model was solved, penalization that does not use adaptive weights. For this reason lasso_weights and gl_weights are None. This function is used mostly along with the cross_validation function that will be introduced in section 3.3.

3.2 WEIGHTS class

The WEIGHTS class includes all the weight calculation methods discussed in Section 2.3. The default parameters from the WEIGHTS class are,

```python
weights = asgl.WEIGHTS(model='lm', penalization='asgl', tau=0.5, weight_technique='pca_pct', weight_tol=1e-4, lasso_power_weight=1, gl_power_weight=1, variability_pct=0.9, lambda1_weights=1e-1, spca_alpha=1e-5, spca_ridge_alpha=1e-2)
```

where the meaning of the arguments is,

- **model**: A string specifying the model to be used when solving non penalized models required in the weights computation. Valid alternatives are:
  - "lm" for solving linear regression models,
  - "qr" for solving quantile regression models,

The model specified here must be the same as in the ASGL class,

- **penalization**: A string specifying the type of penalization to be applied. Valid alternatives are adaptive based ones:
– "alasso" for using an adaptive sparse group lasso penalization,
– "agl" for using an adaptive group lasso penalization,
– "asgl" for using an adaptive sparse group lasso penalization,
– "asgl_lasso" for using an sparse group lasso with adaptive weights in the lasso part,
– "asgl_gl" for using an sparse group lasso with adaptive weights in the group lasso part.

The penalization specified here must be the same as in the ASGL class,

• tau: A floating point number between 0 and 1. Parameter \(\tau\) indicating the quantile level in quantile regression models. Value 0.5 solves the median regression. Value 0.25 solves the first quartile regression. If the model is set to "lm", then tau has no effect. The tau specified here must be the same as in the ASGL class,

• weight_technique: A string indicating the weight technique to use for fitting the adaptive weights. Valid values are:
  – "pca_pct": It computes the weights based on pca using a subset of components,
  – "pca_1": It computes the weights based on pca using the first component,
  – "pls_pct": It computes the weights based on pls using a subset of components,
  – "pls_1": It computes the weights based on pls using the first component,
  – "unpenalized": It computes the weights using a non penalized model. This alternative is only suitable for low dimensional scenarios where the number of observations is larger than the number of variables,
  – "lasso": It computes the weights using a lasso penalized model.
  – "spca": It computes the weights based on sparse pca using a subset of components

• weight_tol: A floating point number, tolerance for a coefficient to be considered as 0,

• lasso_power_weight: A positive floating point number or a list of floating point numbers. It is the parameter \(\gamma_1\) from the penalizations described in Section 2.2 the power at which the lasso weights \(w\) are risen,

• gl_power_weight: A positive floating point number or a list of floating point numbers. It is the parameter \(\gamma_2\) from the penalizations described in Section 2.2 the power at which the group lasso weights \(v\) are risen,
• **variability_pct**: A floating point number between 0 and 1. Percentage of variability explained by pca or pls components used in "pca_pct", "pls_pct" and "spca". Default value is 0.9 meaning that enough coefficients in order to explain up to 90% of the variability are computed. This parameter only affects the weight techniques mentioned here, but has no effect on the rest of the alternatives,

• **lambda1_weights**: A floating point number. The value of the parameter $\lambda$ to be used when computing the weights based on "lasso" weight_technique.

• **spca_alpha**: A floating point number. The value of the alpha parameter in the sparsePCA formulation when using the "spca" weight_technique. The name of the parameter is inherited from the original source in the sklearn package,

• **spca_ridge_alpha**: A floating point number. The value of the ridge_alpha parameter in the sparsePCA formulation when using the "spca" weight_technique. The name of the parameter is inherited from the original source in the sklearn package.

The main function in the WEIGHTS class is *fit*

### 3.2.1 fit function

`fit(x, y, group_index)` function computes the weights for adaptive based penalizations using the information in the WEIGHTS class object. The parameters from this function are the same as for the fit function from ASGL class. Since this function computes adaptive weights, the usual usage of this function (if one is interested on using an adaptive penalization) would require to create a WEIGHTS class object, run the WEIGHTS.fit function, obtain the adaptive weights and pass this adaptive weights as parameters to the lasso_weights and gl_weights parameters from the ASGL class. For example:

```python
>>> weights = asgl.WEIGHTS(
    model="qr", penalization="asgl", tau=0.5,
    lasso_power_weight=[1, 1.2],
    gl_power_weight=[0.7, 0.9, 1.1, 1.3, 1.7])

>>> lasso_weights, gl_weights = weights.fit(x, y, group_index)

>>> model = asgl.ASGL(model="qr", penalization="asgl", tau=0.5,
    lambda1=[0.001, 0.01, 0.1],
    alpha=[0.2, 0.5, 0.7, 0.9],
    lasso_weights=lasso_weights,
    gl_weights=gl_weights)
```
Here the `weights` object, from the `WEIGHTS` class is created. Since the penalization specified is "asgl", by running the `weights.fit` function, the `lasso_weights` and `gl_weights` are computed. Then, an object from the class `ASGL` is created, and the weights computed above are passed as arguments to this object. By calling the function `model.fit`, the quantile regression models with adaptive sparse group lasso penalizations are solved. The penalization parameters are:

- `lambda1`: 3 possible values
- `alpha`: 4 possible values
- `lasso_power_weight`: 2 possible values
- `gl_power_weight`: 5 possible values

Thus, a grid formed of $3 \times 4 \times 2 \times 5 = 120$ values is formed, and 120 models are solved, the results stored in `model.coef_`.

### 3.3 CV class

The `CV` class inherits all the methods from `ASGL` and `WEIGHTS` class and provides methods for performing cross validation in order to find the optimal parameter values. The default parameters from the `CV` class are,

```python
cv = asgl.CV(model, penalization, intercept=True, tol=1e-5, lambda1=1, alpha=0.5, tau=0.5, lasso_weights=None, gl_weights=None, parallel=False, num_cores=None, solver=None, max_iters=500, weight_technique='pca_pct', weight_tol=1e-4, lasso_power_weight=1, gl_power_weight=1, variability_pct=0.9, lambda1_weights=1e-1, spca_alpha=1e-5, spca_ridge_alpha=1e-2, error_type='MSE', random_state=None, nfolds=5)
```
where all the arguments have been already explained in Sections 3.1 and 3.2 except for the last three, directly related with the cross validation process,

- **error_type**: A string indicating the error metric to consider. Valid values are:
  - "MSE": mean squared error,
  - "MAE": mean absolute error,
  - "MDAE": median absolute error,
  - "QRE": quantile regression error,

- **random_state**: An integer number. Seed for the pseudo-random number generation. If a value is provided, it ensures reproducibility of results,

- **nfolds**: An integer number. Number of folds to be used in cross validation.

The main function in the CV class is **cross_validation**

### 3.3.1 Cross Validation Function

cross_validation(x, y, group_index) function performs a cross validation process based on the parameters defined in the CV class object. The parameters in this function are the same as in functions fit from ASGL and WEIGHTS classes: x, y and group_index. The function returns an error matrix of shape (number of models, nfolds). Usage example:

```python
>>> cv_class = asgl.CV(model='qr', penalization='sgl',
                   lambda1=[0.01, 0.1, 1, 10],
                   alpha=[0.1, 0.5, 0.9], parallel=True,
                   tau=0.1, nfolds=10, error_type='QRE',
                   random_state=3)
```

```python
>>> error = cv_class.cross_validation(x, y, group_index)
```

```python
>>> error.shape
(12, 10)
```

First, an object from class CV is created. It stores information for an sparse group lasso quantile regression model to be solved, and considers a grid of 4 possible lambda1 values and 3 possible alpha values, a total number of 12 models. A 10 folds cross validation process is executed, and the result of this process is an error matrix of shape $E \in \mathbb{R}^{12 \times 10}$, where $E_{i,j}$ stores the error value from model $i$ in fold $j$. Additionally, since the random_state has been set to 3, future executions of the same dataset specifying the same random state would return same results, ensuring reproducibility.
3.4 TVT class

The TVT class inherits all the methods from ASGL and WEIGHTS class and provides methods for performing train /validate / test analysis. The default parameters from the CV class are,

```
tvt_class = asgl.TVT(model, penalization, intercept=True, tol=1e-5, lambda1=1, alpha=0.5, tau=0.5, lasso_weights=None, gl_weights=None, parallel=False, num_cores=None, solver=None, max_iters=500, weight_technique='pca_pct', weight_tol=1e-4, lasso_power_weight=1, gl_power_weight=1, variability_pct=0.9, lambda1_weights=1e-1, spca_alpha=1e-5, spca_ridge_alpha=1e-2, error_type='MSE', random_state=None, train_pct=0.05, validate_pct=0.05, train_size=None, validate_size=None)
```

where all the arguments have been already explained in Sections 3.1 and 3.2 except for the last six, directly related with the train /validate / test process,

- **error_type**: A string indicating the error metric to consider. Valid values are:
  - "MSE": mean squared error,
  - "MAE": mean absolute error,
  - "MDAE": median absolute error,
  - "QRE": quantile regression error,

- **random_state**: An integer number. Seed for the pseudo-random number generation. If a value is provided, it ensures reproducibility of results,

- **train_pct**: A floating point number between 0 and 1. Percentage of the dataset to be used for training the model,

- **validate_pct**: A floating point number between 0 and 1. Percentage of the dataset to be used for validating the model,

- **train_size**: An integer number indicating the number of rows from the dataset to be used for training the model. This parameter takes preference over the **train_pct** parameter,

- **validate_size**: An integer number indicating the number of rows from the dataset to be used for validating the model. This parameter takes preference over the **validate_pct** parameter.

The main function in this class is `train_validate_test`
### 3.4.1 train validate test function

The function `train_validate_test(x, y, group_index)` performs a train / validate / test process based on the parameters defined in the `TVT` class object. The parameters from this function are the same as in functions `fit` from `ASGL` and `WEIGHTS` classes. The function returns a Python dictionary containing:

- **optimal_betas**: A 1-dimensional `numpy.ndarray`. The value of the β coefficients that minimized the test error,
- **optimal_parameters**: A Python dictionary containing the value of the parameters with which the optimal solution was achieved,
- **test_error**: A positive floating point number. The value of the test error obtained with the optimal solution.

Usage example:

```python
>>> tvt_class = asgl.TVT(model='qr', penalization='asgl', tau=0.5,
                       lambda1=[0.01, 0.1, 1, 10],
                       alpha=[0.1, 0.5, 0.9],
                       lasso_power_weight=[0.8, 1, 1.2],
                       gl_power_weight=[0.8, 1, 1.2],
                       parallel=True, error_type='QRE',
                       random_state=99, train_size=300,
                       validate_size=200)
>>> tvt_class.train_validate_test(x, y, group_index)

{'optimal_betas':
array([ 2.65930767e+01, 0.00000000e+00, 0.00000000e+00,
       0.00000000e+00, 0.00000000e+00, 0.00000000e+00,
       0.00000000e+00, -5.32798841e-02, 0.00000000e+00,
       0.00000000e+00, -1.52427363e-02, 0.00000000e+00,
       9.51042157e-03, 0.00000000e+00]),
'oatimal_parameters': {'lambda1': 0.01, 'alpha': 0.9, 'lasso_weights':
array([ 3.1650255799, 2.4798156613, 3.3668766214, 7.75672189464, 4.77764968308, 2.8537114713, 1.4044162671, 1.01540062999, 2.352278634, 20.949954, 1.14491563613, 4.453821725, 0.00000000e+00, 0.00000000e+00, 0.00000000e+00, 0.00000000e+00, 0.00000000e+00, 0.00000000e+00, 0.00000000e+00])}
```
First, an object of class TVT is created containing information for solving a quantile regression model with an adaptive sparse group lasso penalization. A train_size=300 is indicated, meaning that 300 rows from the dataset will be used in the training process of the models. A validate_size=200 is indicated. This means that the validation process will be performed using 200 rows from the dataset, and the remaining rows in the dataset \((n - 300 - 200)\) will be used in the test process. The result obtained is a dictionary as described above, containing the value of the optimal \(\beta\) solution, the optimal parameter values, and the test error obtained with this solution.

### 3.5 Extra functions

In addition to the class objects and functions described along this section, the asgl package includes 2 extra functions worth mentioning: `error_calculator` and `train_test_split`.

#### 3.5.1 error calculator function

`error_calculator(y_true, prediction_list, error_type="MSE", tau=None)` is a function that allows to compute the error obtained from a prediction or list of predictions. The parameters of this function are,

- **y_true**: A 1-dimensional `numpy.ndarray` containing the true values of the response variable,
- **prediction_list**: A list of predictions, output from the `ASGL.predict` function described in Section 3.1
- **error_type**: A string indicating the error metric to consider. Valid values are:
  - "MSE": mean squared error,
  - "MAE": mean absolute error,
  - "MDAE": median absolute error,
  - "QRE": quantile regression error,

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• \( \text{tau} \): A floating point number between 0 and 1. Parameter \( \tau \) indicating the quantile level in quantile regression models. This parameter is only used if a quantile regression model was solved.

Usage example:

```python
>>> model = asgl.ASGL(model="lm", penalization="sgl",
lambda1=[0.001, 0.01, 0.1],
alpha=[0.2, 0.5, 0.7])

>>> model.fit(x, y, group_index)

>>> coefficients = model.coef_

>>> predictions = model.predict(x_new=x)

>>> error = asgl.error_calculator(y_true=y,
  prediction_list=predictions)

>>> error

[21.895037097213336, 21.894987951816283, 21.894959521292872,
21.915054953611918, 21.910333713620282, 21.907558654585653,
22.6425078760837, 22.66227036349894, 22.685544907299743]
```

The result is a list of error values of the same length as the `prediction_list`.

### 3.5.2 train test split function

`train_test_split(nrows, train_size=None, train_pct=0.7, random_state=None)`

function randomly generates a train index and a test index to be used on a train / test split. The parameters in this function are:

- \( \text{nrows} \): An integer number. The number of rows in the dataset,

- \( \text{train_size} \): An integer number indicating the number of rows in the dataset that should define the train set,

- \( \text{train_pct} \): A floating point number between 0 and 1 indicating the percentage of the dataset that should be used for training. The parameter \( \text{train_size} \) takes preference over this one,
• **random_state**: An integer number. Seed for the pseudo-random number generation. If a value is provided, it ensures reproducibility of results.

Usage example:

```python
>>> train_idx, test_idx = asgl.train_test_split(
    nrows=10, train_size=7, random_state=5)

>>> train_idx
array([9, 5, 2, 4, 7, 1, 0])
```

In this example a fake `train_idx` of size 7 and a `test_idx` of size 3 are generated for a dataset containing 10 rows.

4 Examples

4.1 Non penalized models

Solving a non penalized linear regression or quantile regression model using the `asgl` package is very simple. In this section, the `BostonHousing` regression dataset, available in the `sklearn` package will be used, so the first step is to import the dataset,

```python
>>> import numpy as np

>>> from sklearn.datasets import load_boston

>>> boston = load_boston()

>>> x = boston.data

>>> y = boston.target
```

After that, the `asgl` package is imported and the dataset is divided into a 70% train set and a 30% test set. Then an object of the class `ASGL` is created containing the information about the model to be solved. In this case, it is only necessary to provide the information for parameters `model` and `penalization`, the latter, in the case of a non penalized model, should be left as `None`. 
>>> import asgl

>>> train_idx, test_idx = asgl.train_test_split(  
    nrows=x.shape[0], train_pct=0.7, random_state=1)

>>> unpenalized_model = asgl.ASGL(model="lm", penalization=None)

>>> unpenalized_model.fit(x=x[train_idx,], y=y[train_idx])

>>> unpenalized_model.coef_

[array([ 3.42867793e+01, -1.20183515e-01, 3.60204868e-02,  
        -1.44737040e-02, 3.11649925e+00, -1.83800932e+01,  
        4.33076482e+00, -1.45478637e-02, -1.58421918e+00,  
        2.99294537e-01, -1.32561898e-02, -9.49536207e-01,  
        9.87429820e-03, -4.29662800e-01])]

Once the coefficients have been obtained, one can compute the predictions and obtain the prediction error easily by calling the `unpenalized_model.predict` and `error_calculator` functions:

>>> predictions = unpenalized_model.predict(x_new=x[test_idx,])

>>> error = asgl.error_calculator(  
    y_true=y[test_idx], prediction_list=predictions,  
    error_type="MSE")

>>> error

[29.450990335365578]

4.2 Sparse group lasso model using cross validation

In this example a high dimensional synthetic dataset generated using the freely available `data-generation` package will be used. This package can easily be installed from the `Python` Package Index repository.

>>> import numpy as np

>>> import data_generation as dgen
>>> data_class = dgen.EqualGroupSize(
    n_obs=1000, group_size=10, num_groups=10, non_zero_groups=5,
    non_zero_coef=6, random_state=1)

>>> x, y, beta, group_index = data_class.data_generation().values()

The dataset generated here contains 1000 observations and 100 variables that are divided into 10 groups of size 10 each. Among these groups, 30 variables are significant (have been used in the calculation of the response variable), and the remaining 70 variables are noise. Using this dataset a quantile regression model with an sparse group lasso penalization will be solved using cross validation.

>>> import asgl

>>> train_idx, test_idx = asgl.train_test_split(
    nrows=x.shape[0], train_pct=0.7, random_state=1)

>>> lambda1 = (10.0 ** np.arange(-3, 1.51, 0.2))

>>> alpha = np.arange(0, 1, 0.05)

>>> cv_class = asgl.CV(model="qr", penalization="sgl",
    lambda1=lambda1, alpha=alpha,
    nfolds=5, error_type="QRE",
    parallel=True, random_state=1)

>>> error = cv_class.cross_validation(x=x[train_idx],
    y=y[train_idx], group_index=group_index)

>>> error.shape

(460, 5)

The synthetic dataset is divided into a train set, in which the cross validation process is executed, and a test set, used for computing the final prediction error. A grid of 23 possible lambda1 values and 20 alpha values is defined, yielding a total number of 460 possible parameter combinations to be solved. parallel is set to True, which means that the cross validation process will be executed in parallel using as many cores as the maximum number available in the machine being used minus 1. A random_state value of 1 is set in order to ensure the reproducibility of this example.
Once the cross validation process is finished, the error obtained in the different models and across different folds is stored in `error`. The mean error across different folds is computed and then the index of the model providing the minimum error value is obtained and stored in `minimum_error_idx`. With this index, the function `retrieve_parameters_value` is used and the value of the parameters minimizing the cross validation error is recovered and stored in `optimal_lambda` and `optimal_alpha`. Now, the final model using just the optimal values obtained above can be computed in order to obtain the test error of this model.

```python
>>> sgl_model = asgl.ASGL(
    model="qr", penalization="sgl", lambda1=optimal_lambda,
    alpha=optimal_alpha)

>>> sgl_model.fit(
    x=x[train_idx, :], y=y[train_idx], group_index=group_index)

>>> final_beta_solution = sgl_model.coef_[0]

>>> final_prediction = sgl_model.predict(x_new=x[test_idx, :])

>>> final_error = asgl.error_calculator(
    y_true=y[test_idx], prediction_list=final_prediction,
    error_type="QRE", tau=0.5)

>>> final_error
[0.6156290699941908]
```

Additionally, given that it is a synthetic dataset, it is possible to compute the true positive rate, a measure of the accuracy of the variable selection comparing the true
beta with the predicted final_beta_solution. First, we remove the intercept from the final_beta_solution,

```python
>>> predicted_beta = final_beta_solution[1:]
```

```python
>>> true_positive = np.sum(
    np.logical_and(np.abs(beta) > 1e-4,
                   np.abs(predicted_beta) > 1e-4))
```

```python
>>> real_positive = np.sum(np.abs(beta) > 1e-4)
```

```python
>>> true_positive_rate = true_positive / real_positive
```

```python
>>> true_positive_rate
1.0
```

A `true_positive_rate` equal to 1 means that 100% of the significant variables were correctly detected as significant.

### 4.3 Adaptive lasso using train / validate / test

For this example, a synthetic dataset will be generated using the `make_regression` function from the `sklearn` package.

```python
>>> import numpy as np
```  
```python
>>> import asgl
```  
```python
>>> import sklearn.datasets
```  
```python
>>> x, y, beta = sklearn.datasets.make_regression(
    n_samples=100, n_features=200,
    n_informative=10, n_targets=1,
    bias=10.0, noise=1.0, shuffle=True,
    coef=True, random_state=1)
```

The above code generates a synthetic dataset formed by 100 observations and 200 variables (a truly high dimensional framework) where only 10 of the variables are significant (used in the computation of the response variable) and the remaining 190 are noise. Using a train
/ validate / test split, an adaptive lasso model is computed. Additionally, a simple lasso model is computed to act as benchmark of the benefits of adaptive models.

```python
>>> lambda1 = 10.0 ** np.arange(-3, 1.51, 0.1)

>>> tvt_lasso = asgl.TVT(
    model='lm', penalization='lasso', lambda1=lambda1,
    parallel=True, error_type='MSE', random_state=1,
    train_size=50, validate_size=25)

>>> lasso_result = tvt_lasso.train_validate_test(x=x, y=y)

>>> lasso_prediction_error = lasso_result['test_error']

>>> lasso_betas = lasso_result['optimal_betas'][1:]

>>> lasso_prediction_error
11.779487290509907
```

The above code performs a train / validate / test optimization of a lasso model using 50 observations in the training process, 25 observations in the validation process and 25 observations in the test process. The optimal betas obtained are stored in `lasso_betas` and the prediction error is stored in `lasso_prediction_error`. Now an adaptive lasso model is solved using a lasso model in the weight computation.

```python
>>> tvt_alasso = asgl.TVT(
    model='lm', penalization='alasso', lambda1=lambda1,
    parallel=True, weight_technique='lasso', error_type='MSE',
    random_state=1, train_size=50, validate_size=25)

>>> alasso_result = tvt_alasso.train_validate_test(x=x, y=y)

>>> alasso_prediction_error = alasso_result['test_error']

>>> alasso_betas = alasso_result['optimal_betas'][1:]

>>> alasso_prediction_error
1.472196185408593
```

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While the solution achieved by the lasso model had a prediction error of 11.77, the solution achieved by the adaptive lasso is 1.47, 8 times smaller. Additionally, it is possible to compute the correct selection rate of both alternatives

```python
>>> def correct_selection_rate(predicted_beta, true_beta):
    true_positive = np.sum(np.logical_and(
        np.abs(true_beta) > 1e-4,
        np.abs(predicted_beta) > 1e-4))
    true_negative = np.sum(np.logical_and(
        np.abs(true_beta) <= 1e-4,
        np.abs(predicted_beta) <= 1e-4))
    correct_selection_rate = \( \frac{\text{true_positive} + \text{true_negative}}{\text{len(true_beta)}} \)
    return correct_selection_rate

>>> lasso_csr = correct_selection_rate(
    predicted_beta=lasso_betas, true_beta=beta)

>>> alasso_csr = correct_selection_rate(
    predicted_beta=alasso_betas, true_beta=beta)

>>> print(f"Lasso correct selection rate: {lasso_csr}")
Adaptive lasso correct selection rate: 1.0
```

While the lasso only selected correctly 13% of the variables, the adaptive lasso was able to correctly select all the variables. Taking as non significant all the non significant variables and taking as significant all the significant variables.

5 Computational details

The results in this paper were obtained using Python 3.8.3 version. All the packages used in this paper are available from the Python Package Index (Pypi) at [https://pypi.org/](https://pypi.org/)
6 Conclusions

In this paper, a Python package called asgl has been introduced. asgl is a powerful package capable of solving linear and quantile regression models using different types of penalizations that, to the best of our knowledge, were not available in any other package or programming language so far. The usage of asgl has been shown throughout three examples detailed in Section 4.

7 Supplementary material

7.1 Installation and requirements

The asgl package is freely available at the Python Package Index (Pypi), one of the best known Python repositories, and can be easily installed by running the command,

\[ \text{pip install asgl} \]

Alternatively, it is possible to directly pull the repository from GitHub and run the setup.py file,

\[ \text{git clone https://github.com/alvaromc317/asgl.git} \]
\[ \text{cd asgl} \]
\[ \text{Python setup.py} \]

The package requires:

- Python (≥ 3.5) programming language version [van Rossum and Drake, 2009],
- scikit-learn (≥ 0.23.1) [Pedregosa et al., 2011], an open source machine learning Python library,
- numpy (≥ 1.15) [Van Der Walt et al., 2011] a package for efficient manipulation of multidimensional arrays,
- cvxpy (≥ 1.1.0) [Diamond and Boyd, 2016], a Python-embedded modeling language for convex optimization problems.
- Additionally, the package makes use of the multiprocessing package, which is not required to be installed, since it is included in the base program.

The package has been mainly tested in Microsoft Windows machines running Windows 10 and Windows 8 versions, as well as in Red Hat Linux machines.
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