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c-lasso - a package for constrained sparse and robust regression and classification in Python

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Summary

This article illustrates c-lasso, a Python package that enables sparse and robust linear regression and classification with linear equality constraints.

The forward model is assumed to be:

$$y = X\beta + \sigma\epsilon \qquad \text{s.t.} \qquad C\beta = 0$$

Here, X and y are given outcome and predictor data. The vector y can be continuous (for regression) or binary (for classification). C is a general constraint matrix. The vector β comprises the unknown coefficients and σ an unknown scale.

Statement of need

The package handles several estimators for inferring location and scale, including the constrained Lasso, the constrained scaled Lasso, and sparse Huber M-estimation with linear equality constraints Several algorithmic strategies, including path and proximal splitting algorithms, are implemented to solve the underlying convex optimization problems. We also include two model selection strategies for determining the sparsity of the model parameters: k-fold cross-validation and stability selection. This package is intended to fill the gap between popular python tools such as `scikit-learn` which cannot solve sparse constrained problems and general-purpose optimization solvers such as `cvx` that do not scale well for the considered problems or are inaccurate. We show several use cases of the package, including an application of sparse log-contrast regression tasks for compositional microbiome data. We also highlight the seamless integration of the solver into `R` via the `reticulate` package.

Current functionalities

Formulations

Depending on the prior on the solution β, σ and on the noise ϵ, the previous forward model can lead to different types of estimation problems.

Our package can solve six of those : four regression-type and two classification-type formulations.

Those are all variants of the standard formulation "*R1*" :

$$\arg\min_{\beta \in \mathbb{R}^d} \|X\beta - y\|^2 + \lambda \|\beta\|_1 \qquad s.t. \qquad C\beta = 0$$

- ***R1* Standard constrained Lasso regression**: This is the standard Lasso problem with linear equality constraints on the β vector. The objective function combines Least-Squares for model fitting with L_1 penalty for sparsity.
- ***R2* Contrained sparse Huber regression**: This regression problem uses the Huber loss as objective function for robust model fitting with L_1 and linear equality constraints on the β vector. The parameter ρ is set to 1.345 by default (Aigner, Amemiya, & Poirier, 1976)
- ***R3* Contrained scaled Lasso regression**: This formulation is similar to *R1* but allows for joint estimation of the (constrained) β vector and the standard deviation σ in a concomitant fashion (P. L. Combettes & Müller, 2020; P. L. Combettes & Müller, 2020). This is the default problem formulation in c-lasso.
- ***R4* Contrained sparse Huber regression with concomitant scale estimation**: This formulation combines *R2* and *R3* to allow robust joint estimation of the (constrained) β vector and the scale σ in a concomitant fashion (P. L. Combettes & Müller, 2020; P. L. Combettes & Müller, 2020).
- ***C1* Contrained sparse classification with Square Hinge loss**: This formulation is similar to *R1* but adapted for classification tasks using the Square Hinge loss with (constrained) sparse β vector estimation (**???**).
- ***C2* Contrained sparse classification with Huberized Square Hinge loss**: This formulation is similar to *C1* but uses the Huberized Square Hinge loss for robust classification with (constrained) sparse β vector estimation (**???**).

Optimization schemes

The available problem formulations *R1*-*C2* require different algorithmic strategies for efficiently solving the underlying optimization problem. We have implemented four algorithms (with provable convergence guarantees) that vary in generality and are not necessarily applicable to all problems. For each problem type, c-lasso has a default algorithm setting that proved to be the fastest in our numerical experiments.

- **Path algorithms (*Path-Alg*)** : This is the default algorithm for non-concomitant problems *R1,R2,C1,C2*. The algorithm uses the fact that the solution path along is piecewise-affine (as shown, e.g., in (Gaines, Kim, & Zhou, 2018)). When Least-Squares is used as objective function, we derive a novel efficient procedure that allows us to also derive the solution for the concomitant problem *R3* along the path with little extra computational overhead.
- **Projected primal-dual splitting method (*P-PDS*)** : This algorithm is derived from (Briceño-Arias & López Rivera, 2019) and belongs to the class of proximal splitting algorithms. It extends the classical Forward-Backward (FB) (aka proximal gradient descent) algorithm to handle an additional linear equality constraint via projection. In the absence of a linear constraint, the method reduces to FB. This method can solve problem *R1*. For the Huber problem *R2*, P-PDS can solve the mean-shift formulation of the problem (see (Mishra & Müller, 2019)).
- **Projection-free primal-dual splitting method (*PF-PDS*)** : This algorithm is a special case of an algorithm proposed in (Combettes & Pesquet, 2011) (Eq.4.5) and also belongs to the class of proximal splitting algorithms. The algorithm does not require projection operators which may be beneficial when C has a more complex structure. In the absence of a linear constraint, the method reduces to the Forward-Backward-Forward scheme. This method can solve problem *R1*. For the Huber problem *R2*, PF-PDS can solve the mean-shift formulation of the problem (see (Mishra & Müller, 2019)).

- **Douglas-Rachford-type splitting method (*DR*)** : This algorithm is the most general algorithm and can solve all regression problems *R1-R4*. It is based on Doulgas Rachford splitting in a higher-dimensional product space. It makes use of the proximity operators of the perspective of the LS objective (see (P. L. Combettes & Müller, 2020; P. L. Combettes & Müller, 2020)) The Huber problem with concomitant scale *R4* is reformulated as scaled Lasso problem with the mean shift (see (Mishra & Müller, 2019)) and thus solved in (n + d) dimensions.

Model selections

Different models are implemented together with the optimization schemes, to overcome the difficulty of choosing the penalization free parameter λ.

- *Fixed Lambda* : This approach is simply letting the user choose the parameter λ, or to choose $l \in [0, 1]$ such that $\lambda = l \times \lambda_{\max}$. The default value is a scale-dependent tuning parameter that has been proposed in [Combettes:2020.2] and derived in (Shi, Zhang, & Li, 2016).
- *Path Computation* :The package also leaves the possibility to us to compute the solution for a range of λ parameters in an interval $[\lambda_{\min}, \lambda_{\max}]$. It can be done using *Path-Alg* or warm-start with any other optimization scheme.
- *Cross Validation* : Then one can use a model selection, to choose the appropriate penalisation. This can be done by using k-fold cross validation to find the best $\lambda \in [\lambda_{\min}, \lambda_{\max}]$ with or without "one-standard-error rule" (see (Hastie, Tibshirani, & Friedman, 2009)).
- *Stability Selection* : Another variable selection model than can be used is stability selection (see [LIN, SHI, FENG, & LI (2014); Meinshausen & Bühlmann (2010); Combettes:2020.2].

Basic workflow

Here is a basic example that shows how to run c-lasso on synthetic data.

c-lasso is available on pip, one can install it using `pip install c_lasso`. Then on python, to import the package, one should use `import classo`

Let us now begin the tutorial. Firstly, let us generate a dataset using the routine `random_data` included in the c-lasso package, that allows you to generate instances using normally distributed data.

```
>>> n,d,d_nonzero,k,sigma =100,100,5,1,0.5
>>> (X,C,y),sol = classo.random_data(n,d,d_nonzero,k,sigma,zerosum=True, seed = 12
>>> list(numpy.nonzero(sol))
[43, 47, 74, 79, 84]
```

This code snippet generates the vectors $\beta \in R^d$, $X \in R^{n \times d}$, $C \in R^{k \times d}$ (here it is actually all-one vector because of the input `zerosum`), and $y \in R^n$ normally distributed with respect to the model $C\beta = 0$, $y - X\beta \sim N(0, \sigma)$ and β has only d_nonzero non-null componant (which are plot exmplicetly above).

Then, let us define a `classo_problem` instance with the generated dataset in order to formulate the optimization problem we want to solve.

```
problem  = classo.classo_problem(X,y,C)  # define a c-lasso problem instance with

problem.formulation.huber  = True
problem.formulation.concomitant = False
problem.formulation.rho = 1.5  # change the formulation of the problem

problem.model_selection.LAMfixed = True # add the computation for a fixed lambda
problem.model_selection.LAMfixedparameters.rescaled_lam = True
problem.model_selection.LAMfixedparameters.lam = 0.1 # lambda is 0.1*lambdamax

problem.model_selection.PATH = True #add the computation of the lambda-path

problem.solve() # solve our optimization problem
```

Here, we have modified the formulation of the problem in order to use *R2*, with $\rho = 1.5$. We have chosen the following model selections : *Fixed Lambda* with $\lambda = 0.1\lambda_{\max}$; *Path computation* and *Stability Selection* which is computed by default. Then, those problems are solved using the method `solve()` which computes everything.

Finally, one can visualize the solutions and see the running time, and the name of the selected variables by calling the instance `problem.solution`. Note that by calling directly the instance `problem` one could also visualize the main parameters of the optimization problems one is solving. In our case, the running time is in the order of 0.1sec for the fixed lambda and path computation, but from 2sec to 4sec for the stability selection computation.

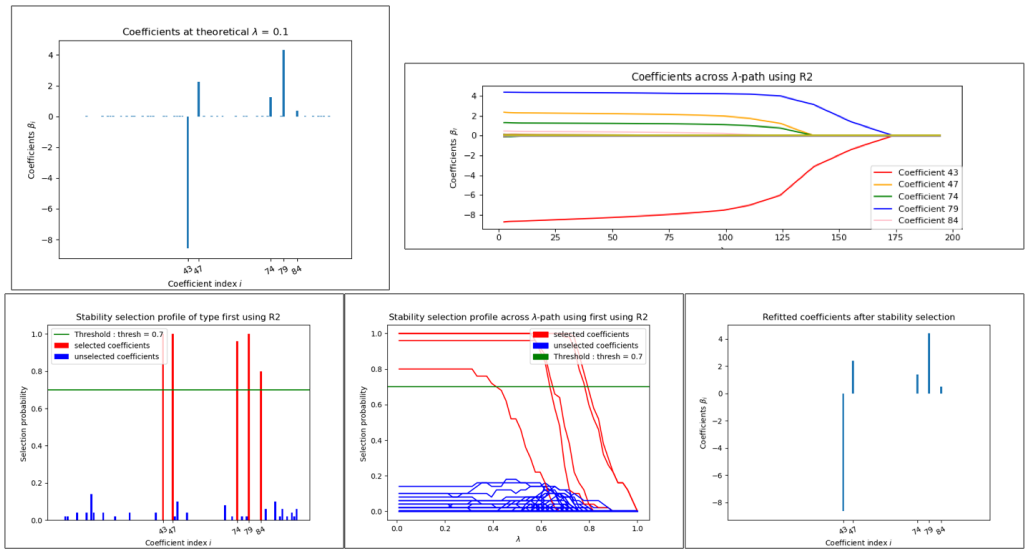

Figure 1: Graphics plotted after calling `problem.solution`

Let us that the models have recovered the right variables and the computation have been done quickly, which is comforting, but not surprising because in this example the noise is little and the number of variable is still small.

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References

Aigner, D. J., Amemiya, T., & Poirier, D. J. (1976). On the estimation of production frontiers: Maximum likelihood estimation of the parameters of a discontinuous density function. *International Economic Review*, *17*(2), 377–396. Retrieved from http://www.jstor.org/stable/2525708

Briceño-Arias, L., & López Rivera, S. (2019). A projected primal–dual method for solving constrained monotone inclusions. *Journal of Optimization Theory and Applications*, *180*(3), 907–924. doi:10.1007/s10957-018-1430-2

Combettes, P. L., & Müller, C. L. (2020). Perspective maximum likelihood-type estimation via proximal decomposition. *Electron. J. Statist.*, *14*(1), 207–238. doi:10.1214/19-EJS1662

Combettes, P. L., & Müller, C. L. (2020). Regression models for compositional data: General log-contrast formulations, proximal optimization, and microbiome data applications. *Statistics in Biosciences*. doi:10.1007/s12561-020-09283-2

Combettes, P., & Pesquet, J.-C. (2011). Primal-dual splitting algorithm for solving inclusions with mixtures of composite, lipschitzian, and parallel-sum type monotone operators. *Set-Valued and Variational Analysis*, *20*, 1–24. doi:10.1007/s11228-011-0191-y

Gaines, B. R., Kim, J., & Zhou, H. (2018). Algorithms for fitting the constrained lasso. *Journal of Computational and Graphical Statistics*, *27*(4), 861–871. doi:10.1080/10618600.2018.1473777

Hastie, T., Tibshirani, R., & Friedman, J. H. (2009). *The elements of statistical learning: Data mining, inference, and prediction*. Springer series in statistics. Springer. ISBN: 9780387848846

LIN, W., SHI, P., FENG, R., & LI, H. (2014). Variable selection in regression with compositional covariates. *Biometrika*, *101*(4), 785–797. Retrieved from http://www.jstor.org/stable/43304688

Meinshausen, N., & Bühlmann, P. (2010). Stability selection. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, *72*(4), 417–473. doi:10.1111/j.1467-9868.2010.00740.x

Mishra, A., & Müller, C. (2019). Robust regression with compositional covariates.

Shi, P., Zhang, A., & Li, H. (2016). Regression analysis for microbiome compositional data. *Ann. Appl. Stat.*, *10*(2), 1019–1040. doi:10.1214/16-AOAS928