LASSO extensions

BIOS 8040

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2022-01-31

LASSO review

- Data: $(\mathbf{x}_i, y_i)$ where $\mathbf{x}_i = (x_{i1}, \ldots, x_{ip})'$ are the predictor values; y_i are the (independent) response values; and $i = 1, \ldots, n$.
- Let $\hat{\beta}_0 \in \mathbb{R}$ and $\hat{\boldsymbol{\beta}} = \left(\hat{\beta}_1, \ldots, \hat{\beta}_n\right)'$, the LASSO estimator is

$$\left(\hat{\beta}_0, \hat{\boldsymbol{\beta}}\right) = \underset{\beta_0, \boldsymbol{\beta}}{\arg\min} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \mathbf{x}_i' \boldsymbol{\beta}\right)^2 \right\} \quad \text{s. t.} \sum_{j=1}^{p} |\beta_j| \leq t,$$

- or equivalently,

$$\left(\hat{\beta}_0, \hat{\boldsymbol{\beta}}\right) = \underset{\beta_0, \boldsymbol{\beta}}{\arg\min} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \mathbf{x}_i' \boldsymbol{\beta}\right)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right\}.$$

[1] Tibshirani R. Regression shrinkage and selection via the LASSO, 1995. JR Stat Soc B 58:1 267-288.
[2] Friedman J, et al. Regularization paths for generalized linear models via coordinate descent, 2010. J Stat Soft, 33:1.

Some issues with LASSO and what I'll be talking about today

Elastic net

Motivation

- Ridge regression and LASSO both perform well under different circumstances. In particular, ridge seems (empirically) to always win if many variables are correlated.
- Why? LASSO **tends to select only one of a set of correlated predictors.** The choice is unstable under small perturbations.
- LASSO can only select n predictors (bad when $p \gg n$).
- **Solution**: combine L1 penalty of LASSO with L2 penalty of ridge.
- As an added benefit, elastic net also tends to be at worst equal with LASSO in terms of prediction error.

[1] Tibshirani R, 1995. JR Stat Soc B, 58:1 267-288.
[3] Zou H & Hastie T, Regularization and variable selection via the elastic net, 2005. JR Stat Soc B, 67:2 301-320.

Naive loss function

- We can combine the two penalty terms to write a new loss function:

$$\left(\hat{\beta}_0, \hat{\boldsymbol{\beta}}\right) = \underset{\beta_0, \boldsymbol{\beta}}{\arg\min} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \mathbf{x_i}'\boldsymbol{\beta}\right)^2 + \lambda_1 \sum_{j=1}^{p} |\beta_j| + \lambda_2 \sum_{j=1}^{p} \beta_j^2 \right\}.$$

- Zou and Hastie use the matrix notation. But this is equivalent.
- Let's reparametrize the penalty term: let $\alpha = \frac{\lambda_2}{\lambda_1 + \lambda_2}$. Then we can write

$$\left(\hat{\beta}_0, \hat{\boldsymbol{\beta}}\right) = \underset{\beta_0, \boldsymbol{\beta}}{\arg\min} \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \mathbf{x_i}'\boldsymbol{\beta}\right)^2 + \lambda P\left(\alpha, \boldsymbol{\beta}\right) \right\}.$$

- Here, $P(\alpha, \boldsymbol{\beta}) = (1 - \alpha) \sum_{j=1}^{p} |\beta_j| + \alpha \sum_{j=1}^{p} \beta_j^2$ and $\lambda \in \mathbb{R}$.

Geometry (Tibshirani 1996)

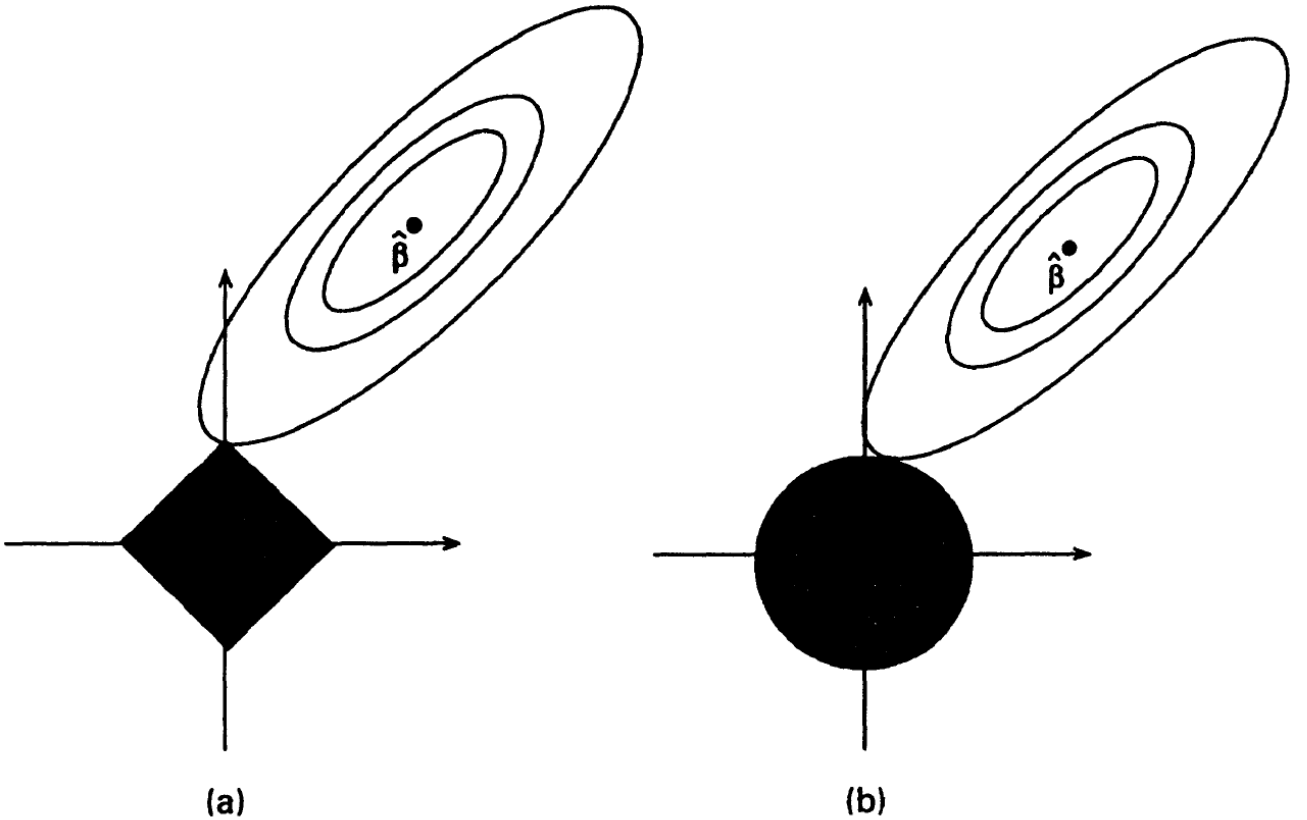


Fig. 2. Estimation picture for (a) the lasso and (b) ridge regression

Geometry (Zou & Hastie 2005)

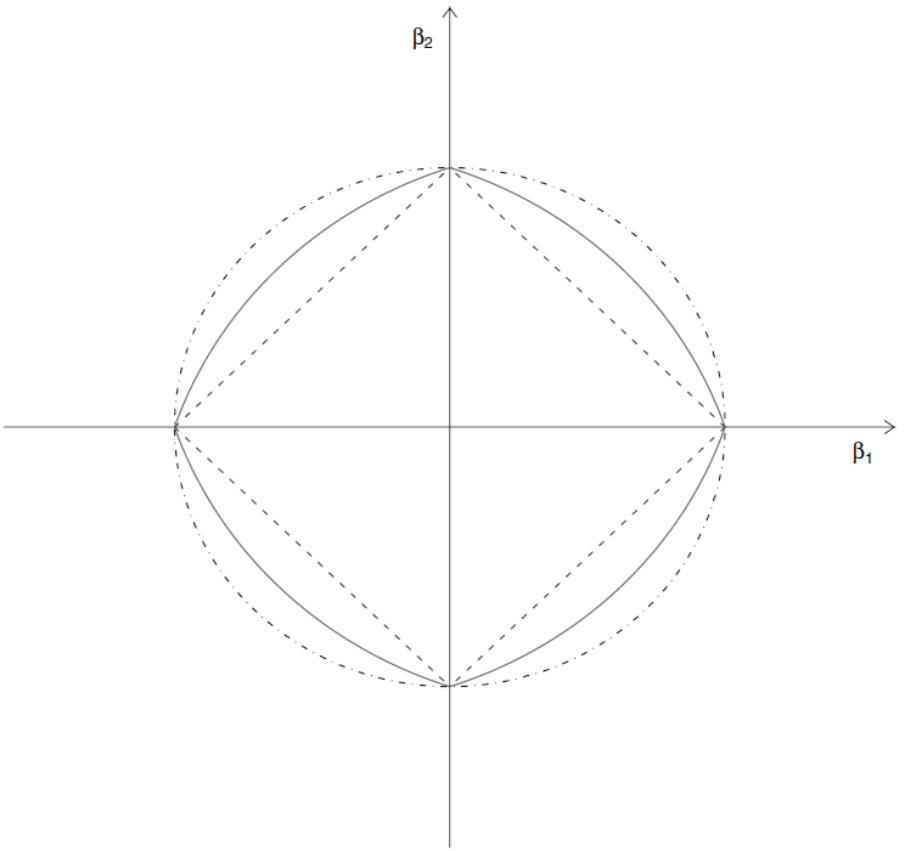


Fig. 1. Two-dimensional contour plots (level 1) (· - · - · -, shape of the ridge penalty; -------, contour of the lasso penalty; ———, contour of the elastic net penalty with $\alpha = 0.5$): we see that singularities at the vertices and the edges are strictly convex; the strength of convexity varies with α

Theoretical advantages of this loss function:

- The modified penalty allows for a **grouping effect**.
- Elastic net tends to include **all predictors in a highly correlated subset**, and then continuously shrinks the coefficients.

Empirical concerns:

- Hastie and Zou suggest that this naive loss function appears to perform badly if α is far from 0 (LASSO) or 1 (ridge).
- They provide some empirical evidence of this, but not much. They suggest this is due to "double shrinkage".
- Suggestion is to rescale solution by a factor of $1 + \lambda_2 = 1 + \lambda(1 - \alpha)$.

Maybe naive is fine, actually? ¯\(ツ)/¯

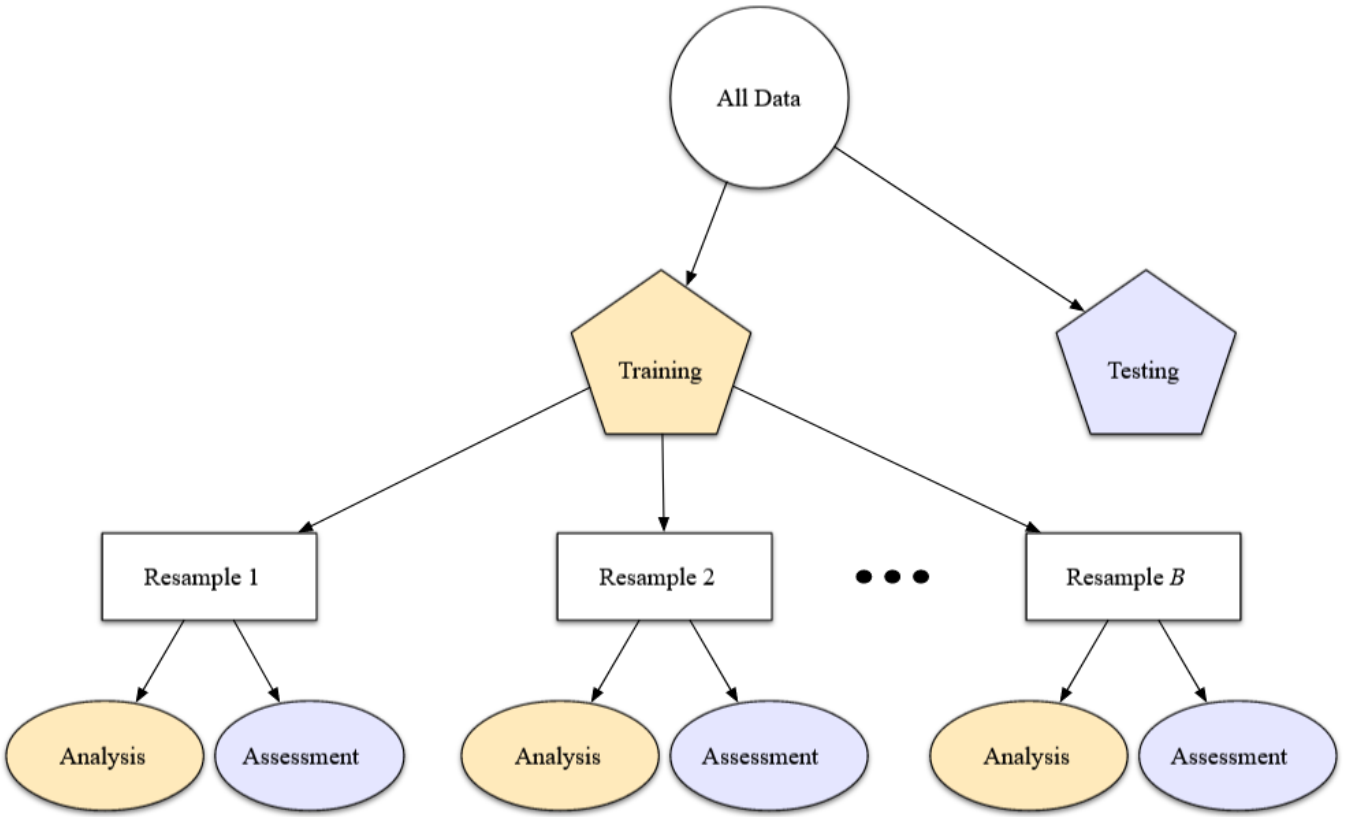
- According to this Cross Validated post, Hastie now recommends the **relaxed LASSO** approach instead.
- In the original paper describing the relaxed LASSO [4], the relaxed LASSO estimator is estimated from running LASSO twice in a row: once on all predictors, and again on the subset of included predictors (with a new penalty term).
- In Hastie's `glmnet` package [5] he uses this relaxation method: let $\hat{\boldsymbol{\eta}}_\lambda$ be the fitted linear predictor with penalty λ, and let $\tilde{\boldsymbol{\eta}}_\lambda$ be the OLS linear predictor using **only the variables from the active set.**
- The rescaled linear predictor is then

$$\tilde{\boldsymbol{\eta}}_{\gamma,\lambda} = (1-\gamma)\tilde{\boldsymbol{\eta}}_\lambda + \gamma\hat{\boldsymbol{\eta}}_\lambda.$$

[4] Meinshausen N, Relaxed lasso, 2007. Comp Stat & Data Analysis, 52:1, 374-393.

[5] https://glmnet.stanford.edu/articles/relax.html

Practical issue: choosing λ and α (and γ)



(Figure from Tidy Modeling with R, cp. 10 by Max Kuhn and Julia Silge.)

Practical issue: choosing λ and α (and γ)

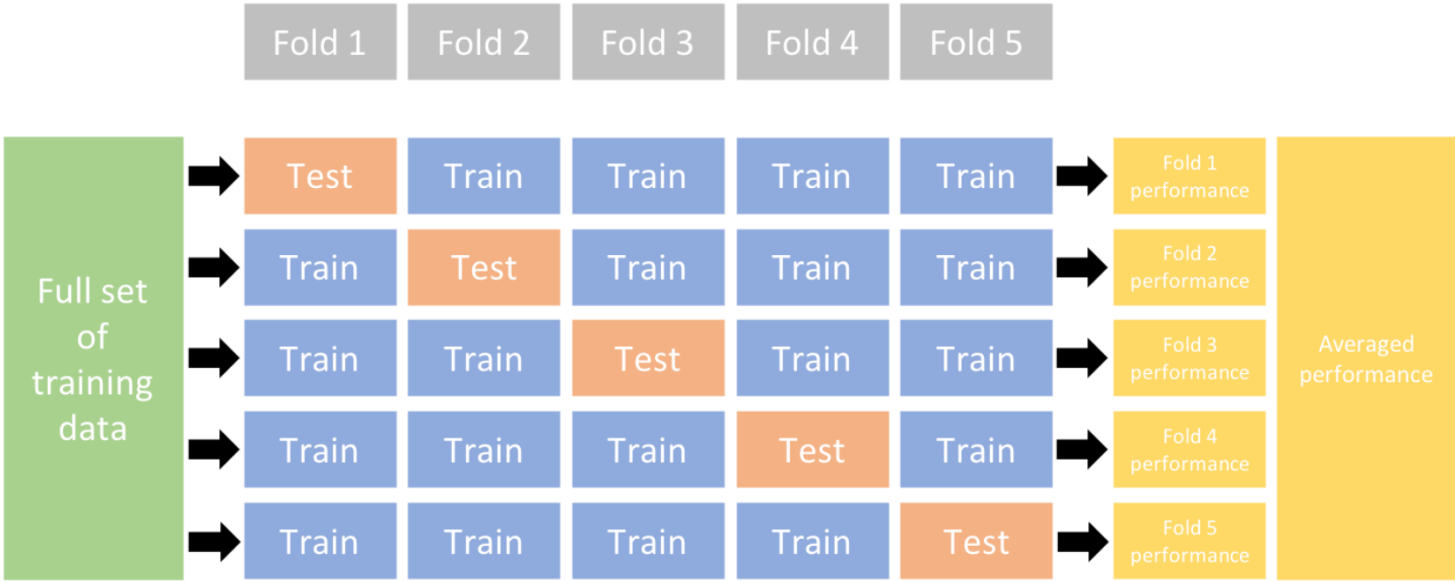


Figure 2.4: Illustration of the k-fold cross validation process.

(Figure from Hands-On Machine Learning with R, cp. 2 by Bradley Boehmke and Brandon Greenwell.)

Additionally, this is also repeated multiple times and averaged.

Adaptive LASSO

The variable selection problem

- Given a response variable $\mathbf{y} \in \mathbb{R}^n$ and some set of $p$linearly independent predictor variables, $X = [\mathbf{x}_1, \ldots, \mathbf{x}_p] \in \mathbb{R}^{n \times p}$, assume that

$$E[y \mid x] = \beta_1 x_1 + \ldots + \beta_p x_p.$$

- Further, suppose $\mathcal{A} = \{j : \beta_j \neq 0\}$ s.t. $|\mathcal{A}| = p_0 < p$.

- We use some procedure δ which gives the estimator $\hat{\boldsymbol{\beta}}(\delta)$.
  Define $\mathcal{A}(\delta) = \{j : \hat{\beta}_j \neq 0\}$.

- We want to know whether $\mathcal{A}(\delta) = \mathcal{A}$ is true. That is, is the selected active set of predictors the same as the **true** active set of predictors?

The statistician (right) consults the oracle (left) about the true predictor set. Source link.

What can we do if the oracle is out? Source link.

The oracle

- An **oracle** procedure would know the true contents of $\mathcal{A}$ prior to estimation. In the real world, this is impossible, so we have to be content with procedures that have the **oracle property**.
- We call a procedure δ an **oracle** if:

1. $\hat{\boldsymbol{\beta}}(\delta)$ identifies the correct subset model, i.e. $\mathcal{A}(\delta) = \mathcal{A}$.
2. $\hat{\boldsymbol{\beta}}(\delta)$ is asymptotically normal, that is, given true covariance matrix $\boldsymbol{\Sigma}$,

$$\sqrt{n}\left(\hat{\boldsymbol{\beta}}(\delta)_{\mathcal{A}} - \boldsymbol{\beta}_{\mathcal{A}}\right) \xrightarrow{d} \mathcal{N}\left(\mathbf{0}, \boldsymbol{\Sigma}\right).$$

[6] Zou H, The adaptive lasso and its oracle properties, 2006. JASA 101:476 1418 - 1429.

Is the LASSO an oracle?

- Fan and Li (2001): bias of LASSO estimates leads to conjecture that LASSO is not an oracle. Suggest SCAD as an oracle.
- Zou cites several papers which show consistency in variable selection under certain conditions (1, 2,3, a fourth paper that is unavailable anywhere online 🙄).
- Frank Harrell tweets about this a lot. In general his argument is that LASSO/EN is unstable, and thus cannot be consistent.
- He recommends this review paper. In general, concludes that with current λ selection methods, the oracle property is not attained.
- In general, it is easy to show that the LASSO cannot have the oracle property in the general case by simulating data and fitting the model.
- Zou concludes that LASSO is only guaranteed to be consistent in simple cases, such as orthogonal design, and when $p = 2$. Both cases still require correct choice of λ.

The adaptive LASSO

- Lasso estimator with weighting:

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} \left(y_i - \mathbf{x_i}' \boldsymbol{\beta} \right)^2 + \lambda \sum_{j=1}^{p} w_j \left| \beta_j \right| \right\}$$

- **Key idea:** different penalties can be applied to each coefficient.
- **If weights are chosen cleverly, the weighted LASSO can be an oracle.**
- Zou's choice of weights: let $\hat{\boldsymbol{\beta}}$ be a root-n consistent estimator of $\boldsymbol{\beta}^*$, such as from OLS. Pick $\gamma > 0$, then define

$$\hat{w}_j = \frac{1}{|\hat{\beta}_j^*|^\gamma}.$$

- Now, with the correct choice of λ, the adaptive LASSO has the oracle properties.

Important note

- I think the oracle property is interesting in theory, but there is still no guarantee that an oracle procedure will always find the true model. **Our sample size is not infinite.**
- Frank Harrell (my hero) agrees with me that using an oracle estimator doesn't necessarily mean anything in practice.
- If anyone is looking for a good research project, maybe look into the relationship between n and selection of the true model - Zou uses a framework that could be interesting.

Group LASSO

Motivation

- Suppose you have a response, y, and two categorical predictors, x_1 and x_2, which both have 3 levels. You dummy code your covariates and end up with four predictors, say $x_{12}, x_{13}, x_{22}, x_{23}$.
- You fit a linear model using LASSO, and you get non-zero estimates for x_{12} and x_{23}. Does this make any sense? It would be better to include both x_{12} AND x_{13} or neither of them.
- Yuan and Lin also suggest that LASSO tends to include more factor variables than necessary, and that changes in factor representation change variable selection (this is unsurprising).

[7] Yuan M & Lin Y, Model selection and estimation in regression with grouped variables, 2006. JR Stat Soc B 68:1 49-67.

Definition

- Given positive definite matrices $K_1, \ldots, K_J$; the group LASSO estimator is defined (by Yuan and Lin) as

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} \left(y_i - \mathbf{x_i}' \boldsymbol{\beta} \right)^2 + \lambda \sum_{j=1}^{J} \left(\boldsymbol{\beta}' K_j \boldsymbol{\beta} \right)^{1/2} \right\}.$$

- To see how this is similar to the previous penalty terms, set $K_j = I_{p_j}$ for all j. Then we can write

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} \left(y_i - \mathbf{x_i}' \boldsymbol{\beta} \right)^2 + \lambda \sum_{j=1}^{J} \left(\sum_{k=1}^{p_j} \beta_k^2 \right) \right\}.$$

- Setting K_j to be anything else results in weighting--Yao and Lin suggest $K_j = p_j I_p$, but don't really give any good reasons.

- This corresponds to L1 penalty between groups, and L2 penalty within groups. (see Fig 1 in paper.)

The opposite idea: exclusive LASSO

- Define the exclusive LASSO estimator as

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} \left(y_i - \mathbf{x_i}' \boldsymbol{\beta} \right)^2 + \lambda \sum_{j=1}^{J} \left(\sum_{k=1}^{p_j} |\beta_k| \right)^2 \right\}.$$

- If we add (unnecessary) absolute value bars to the group LASSO estimator, you can really see how they are opposites:

$$\hat{\boldsymbol{\beta}} = \arg\min_{\boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} \left(y_i - \mathbf{x_i}' \boldsymbol{\beta} \right)^2 + \lambda \sum_{j=1}^{J} \left| \sum_{k=1}^{p_j} \beta_k^2 \right| \right\}.$$

[8] Zhou Y et al., Exclusive lasso for multi-task feature selection, 2010. Proceedings of the 13th International Conference on Artificial Intelligence and Statistics.
[9] Campbell F and Allen G, Within group variable selection through the exclusive lasso, 2017. Elec J Stats 11 4220-42257.
[10] Qiu L et al., Exclusive lasso based k-nearest-neighbor classification, 2021. Neural Computing and Applications.

3D geometry of group/exclusive LASSO

- Fig 1 from Yuan and Lin - group LASSO
- Fig 1 from Campell and Allen - exclusive LASSO
- These two penalty functions belong to a set of "CAP" penalties that generalize hierarchical structure for regularization penalties.

Implementation

- The 'industry-standard' implementation of elastic net and adaptive LASSO is with `glmnet`.
- The `tidymodels` infrastructure makes some practical considerations easier. Currently doesn't support group/elastic/adaptive lasso.
- AFAIK, there is no automated version implementation Zou's procedure for estimating weights that is current and well-tested.
- The `gcdnet` package is powerful and performant, but is poorly documented and not mature.
- Group lasso can be implemented in R with `grplasso` or `gglasso`. Exclusive lasso can be implemented with `ExclusiveLasso`.
- I have some examples ready in another doc that I will switch to now.

Final notes

- In theory, it should be possible to have a relaxed adaptive group elastic net estimator. But all of these combinations may not be implemented - if you need to combine features, it is best to think about what is most important.
- Important to remember that even an oracle method cannot always generate the true, causal model. LASSO-type methods are better for prediction and hypothesis generation than they are for causal inference and hypothesis confirmation.