

Data Analysis and Model Classification

Guidesheet VIII: Regularized regression

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Introduction



At this point of the course, you should already learned that problems can occur when trying to train models with many parameters with a few samples. In this guidesheet, you will learn techniques to train regression models, specifically using regularization terms based on L_1 and L_2 normalization constraints. As last week, we will use the mean square error (MSE, `immse` in MATLAB) to evaluate our models. For this we will use only 5% of the samples for training and the rest for testing. This is not a smart design choice, but we will use it here for pedagogical purposes to clearly understand the concept of regularization and its effects when data is scarce.

The L_2 norm is nothing else than the euclidian norm, defined as $\|x\|_2 = \sqrt{\sum_{i=1}^p x_i^2}$, where p is the dimension of the vector $x = [x_1, \dots, x_p]^T$. The L_1 norm is the sum of the absolute values of each elements of the vector x : $\|x\|_1 = \sum_{i=1}^p |x_i|$. You can use the MATLAB commands `norm(x,1)` and `norm(x,2)` to compute these L_1 and L_2 norms.

Regression

The parameters of the standard regression are found through error minimization; specifically by solving $\min_{\beta} \|y - X\beta - \beta_0\|_2$ minimization where y are the labels (`PosX` and `PosY`), X is the training data and β is the vector of regression coefficients, with β_0 being the *intercept* (bias).

Hands on

- Apply regression without PCA. Use linear regression with an intercept ($X=[I \text{ FM}]$, where I is a vector of 1s and FM the feature matrix/training data) and compute the test error (as you did last week). Is it a good mean square error? Plot the output compared to the labels. 
- How many parameters do you have to estimate when using regression in this problem? Compare the number of parameters to the number of samples available for training. 

LASSO



LASSO adds a L_1 regularization constraint to the definition of the regression coefficients:

$$\min_{\beta} \|y - X\beta - \beta_0\|_2 \quad s.t. \quad \lambda \|\beta\|_1 \leq 1 \quad (1)$$

The constraint means that the L_1 norm of the weight vector (β) times λ must not exceed 1 (meaning that the norm must not exceed $\frac{1}{\lambda}$). This regularization type leads to sparse weight vectors (meaning that a lot of the coefficients will be zeros). The larger the λ , the sparser the resulting solution will become.

MATLAB provides the `lasso` function, and includes a cross-validation option to automatically select the λ that gives the smallest cross-validation (mean square) error. Have a (thorough) look at the MATLAB help for this function. Use a 10-fold cross-validation and set the hyperparameter `lambda = logspace(-10,0,15)` for example. The `lasso` function takes care of adding the intercept so you can feed it the training data directly. The function outputs two variables: `B` and `FitInfo`. `B` is a matrix containing the regression weights for all λ s. The `FitInfo` structure contains the intercept and the mean square error (MSE) for each λ .

Hands on

- Apply LASSO on the training data. For each λ value, what is the number of non zero β weights? How does this number change as λ increases? 
- Plot the cross-validation MSE for each λ and interpret it. For better visualization you can use a logarithmic scale using `semilogx(lambda,FitInfo.MSE)`.
- For the λ value corresponding to the best MSE, use the corresponding β and *intercept* to regress the test data (`PosX`, `PosY`). Plot the data and compute the test MSE. Happy? 


Elastic nets

LASSO has two limitations: firstly, when $N < p$, it only sets a maximum of N out of p weights to a non-zero value (N : number of samples and p : number of features). This is not so much of a problem in our example, since p is not so much larger than N , but can be problematic, when $N \ll p$. The second limitation is much more problematic in our case: when groups of features are correlated, LASSO will only select one of these features since it optimizes sparsity. To cope with these limitations, we can add a second constrain on the L_2 norm. This method is called Elastic nets. The two constrains will be weighted by an additional factor $0 < \alpha \leq 1$:

$$c(\beta) = \alpha \|\beta\|_1 + \frac{1 - \alpha}{2} \|\beta\|_2^2 \quad (2)$$

You can see that when $\alpha = 1$, elastic nets reduce to LASSO. Use the same parameters as in the previous section, except for $\alpha = 0.5$ instead of 1. Of course, α is also a *hyperparameter*. What is the appropriate way to set it up?

Hands on

- Apply an elastic net on the training data, choose the relevant arguments for the `lasso` function. Use For each λ value, what is the number of non zero β weights? How does it evolve with λ increasing. For each λ value, compare the number of non-zero weights between LASSO and elastic nets. 
- For the λ value corresponding to the best MSE, use the corresponding β and *intercept* to regress the test data (`PosX`, `PosY`). Plot the data and compute the test MSE. Again, compare with the last section.
- Optimize your hyperparameters. Will you use a cross-validation or a single training-test split? How will you estimate performance of a model which optimizes hyperparameters? 