L1L2Py Documentation

Release 1.0.5

Salvatore Masecchia

January 25, 2012

CONTENTS

Release
1.0.5

Date
January 25, 2012

Homepage
http://slipguru.disi.unige.it/Software/L1L2Py

Download
http://slipguru.disi.unige.it/Software/L1L2Py/L1L2Py-1.0.5.tar.gz

L1L2Py is a Python package to perform feature selection by means of $\ell_1\ell_2$ regularization with double optimization.

L1L2Py makes use of NumPy to provide fast N-dimensional array manipulation. It is licensed under GNU General Public License (GPL) version 3.

L1L2Py is based on the minimization of the (naive) $\ell_1\ell_2$ functional introduced in [Zou05] using the algorithm studied from the theoretical viewpoint in [DeMol09a]. The current implementation exploits the minimization algorithm proposed in [Beck09].

L1L2Py is the Python implementation of the one proposed and applied in [DeMol09b]. It consists of two stages. The first one identifies the minimal set of relevant variables (in terms of prediction error). Starting from the minimal list, the second stage selects the family of (almost completely) nested lists of relevant variables for increasing values of linear correlation.

CHAPTER

ONE

GETTING STARTED

L1L2Py is a simple and lightweight python package to perform variable selection. The algoritms proposed and implemented are been well studied in different experimental settings.

The package is self contained and gives all the needed tools to generate sparse solution for a given linear classification or regression problem.

1.1 Installation

L1L2Py is available open-source under the GNU GPL license. It requires Python version 2.5 or higher and the NumPy package.

There are two ways you can get it:

- **Automatic Installation (recomended)**

  L1L2Py is available on the Python Package Index and can be installed via easy-install

  ```
  $ easy_install -U L1L2Py
  ```

  or pip

  ```
  $ pip install -U L1L2Py
  ```

- **Manual Installation**

  Download the latest official version L1L2Py-1.0.5.tar.gz, then:

  ```
  $ tar xzvf L1L2Py-1.0.5.tar.gz
  $ cd L1L2Py-1.0.5
  $ python setup.py install
  ```

  Using this manual installation, if the testing framework Nose is installed, is possible to run the given Unit Test running the `nosetests` script

  ```
  $ nosetests
  ..................................
  ----------------------------------------------------------------------
  Ran 36 tests in 3.002s

  OK
  ```

Moreover, in order to generate the plots showed in the following tutorial the Matplotlib package (with the mplot3d toolkit enabled) is required.

1.2 Tutorial

This tutorial aims to show how the $\ell_1\ell_2$ regularization with double optimization is able to perform variable selection. Moreover, the tutorial shows how to use L1L2Py on a synthetic dataset generated with a given function which simulates a linear regression problem with a subset of relevant and linearly correlated variables.

Even if it's not mandatory, in order to better understand this tutorial the reader should read the method described in [DeMol09b], or at least the introduction of *Main functions (l1l2py)*.

1.2.1 Synthetic Data Generation

Using the script `dataset_generation.py` (`L1L2Py-1.0.5/docs/tutorial/dataset_generation.py`), synthetic data can be generated for a supervised regression problem. The script contains a function (called `correlated_dataset`) which generates a data matrix with some relevant, correlated and noisy variables.

Running the script with only two parameters (i.e. the data matrix dimensions) two text files, namely `data.txt` and `labels.txt` are generated in the same directory containing the script file.

```
$ python dataset_generation.py 100 40
Generation of 100 samples with 40 variables... done
$ ls
dataset_generation.py  data.txt  labels.txt
```

The script generates a random dataset with **3 groups of 5 correlated variables**. In total, there are **15 relevant variables** and, following the example above, *40* - *15* = **25 noisy variables**. The weight assigned to each relevant variable is *1.0*.

The `data matrix` and the `labels matrix` generated with the script and used in this tutorial can be found in the the directory `L1L2py-1.0.5/docs/tutorial`), where the script itself is located.

To familiarize with the `l1l2py` code, the two files can be copied where needed and used following the tutorial steps below (alternatively, different datasets can be generated using either the script or the function `correlated_dataset`).

1.2.2 Preparing the data

First, starting a new python terminal, import the needed packages:

```
>>> import numpy as np
>>> import l1l2py
```

and load the data from disk (change file paths as needed):

```
>>> X = np.loadtxt('tutorial/data.txt')
>>> Y = np.loadtxt('tutorial/labels.txt')
```

Then, split the data in two blocks, training-set and test-set using the standard NumPy functions `numpy.vsplit` and `numpy.hsplit`

```
>>> train_data, test_data = np.vsplit(X, 2)
>>> print train_data.shape, test_data.shape
(50, 40) (50, 40)
>>> train_labels, test_labels = np.hsplit(Y, 2)
>>> print train_labels.shape, test_labels.shape
(50,) (50,)
```

as shown, each set contains *50* samples.

1.2.3 Setting parameters ranges

At this point a correct range for the regularization parameters has to be chosen. The function `l1l2py.algorithms.l1_bound` can be used to devise an optimal range for the sparsity parameter τ.

```
>>> train_data_centered = l1l2py.tools.center(train_data)
>>> tau_max = l1l2py.algorithms.l1_bound(train_data_centered, train_labels)
>>> print tau_max
10.5458157567
```

Note that the matrix is centered, because the same normalization will be used when running the model selection procedure (see later).

Using this parameter to solve a *Lasso* optimization problem, a void solution would be obtained:

```
>>> beta = l1l2py.algorithms.l1l2_regularization(train_data_centered,
...                                              train_labels, 0.0, tau_max)
>>> print np.allclose(np.zeros_like(beta), beta)
True
```

A good choice for the extreme values for τ could be

```
>>> tau_max = tau_max - 1e-2
>>> tau_min = tau_max * 1e-2
>>> beta_max = l1l2py.algorithms.l1l2_regularization(train_data_centered,
...                                                  train_labels, 0.0, tau_max)
>>> beta_min = l1l2py.algorithms.l1l2_regularization(train_data_centered,
...                                                  train_labels, 0.0, tau_min)
>>> print len(beta_max.nonzero()[0]), len(beta_min.nonzero()[0])
1 10
```

The minimum value of τ should be set in order to get a solution with more non-zero variables than the number of *hypotetical* number of relevant groups of correlated variables (in the our case we know to have *3* groups).

The range of τ values can therefore be set as:

```
>>> tau_range = l1l2py.tools.geometric_range(tau_min, tau_max, 20)
```

For the regularization parameter λ a wide range of values is advisable

```
>>> lambda_range = l1l2py.tools.geometric_range(1e-6, 1e-3, 7)
```

as for the correlation parameter μ. For this simple example some different levels of correlation are set, starting from *0.0*

```
>>> mu_range = [0.0, 0.001, 0.01, 0.1, 1.0]
```

1.2.4 Run the model selection

To correctly use the *Stage I: Minimal Model Selection*, cross validation splits must be generated:

```
>>> cv_splits = l1l2py.tools.kfold_splits(train_labels, k=5) #5-fold CV
```

Now, call the `l1l2py.model_selection` function to get the results of model selection (the complete execution of the function will take some minutes)

```
>>> out = l1l2py.model_selection(train_data, train_labels,
...                              test_data, test_labels,
...                              mu_range, tau_range, lambda_range,
...                              cv_splits,
...                              cv_error_function=l1l2py.tools.regression_error,
...                              error_function=l1l2py.tools.regression_error,
...                              data_normalizer=l1l2py.tools.center,
...                              labels_normalizer=None)
```

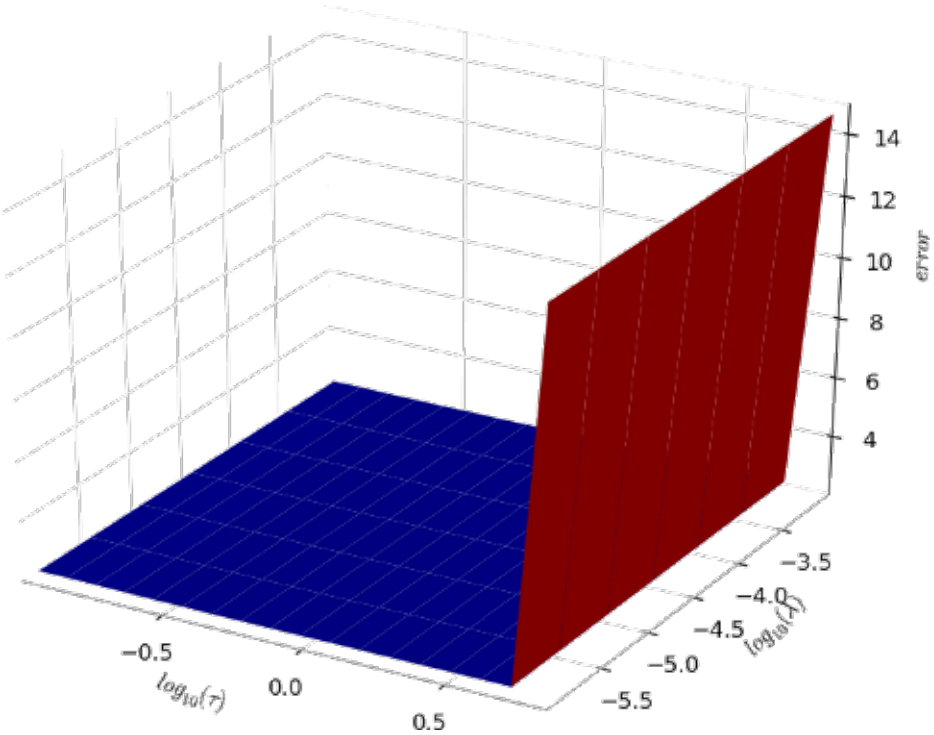
1.2.5 Analyze the results

The optimal value of τ and λ found in the *Stage I: Minimal Model Selection* are:

```
>>> print out['tau_opt'], out['lambda_opt']
0.451073293459 0.000316227766017
```

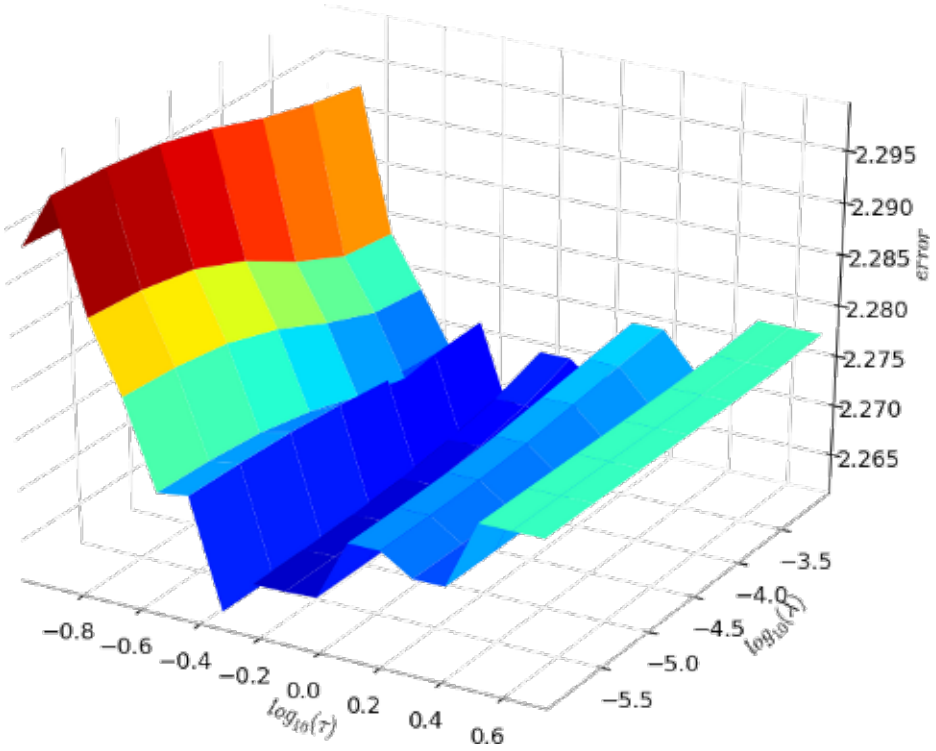
The module `plot.py` (`L1L2py-1.0.5/docs/tutorial/plot.py`), provides a function (called `kcv_errors`) to plot the mean cross validation error (remember that for some high values of τ, the solution could be void on some cross validation splits, see *Stage I: Minimal Model Selection*, so the mean could be evaluated on a subset of (τ, λ) pairs)

```
>>> from matplotlib import pyplot as plt
>>> from plot import kcv_errors
>>> tau_max_idx = out['kcv_err_ts'].shape[0]
>>> kcv_errors(out['kcv_err_ts'],
...            np.log10(tau_range[:tau_max_idx]), np.log10(lambda_range),
...            r'$log_{10}(\tau)$', r'$log_{10}(\lambda)$')
>>> plt.show()
```



Since the error increases rapidly with the highest value of τ, is useful to show the error surface removing the (corresponding) last row from the mean errors matrix

```
>>> tau_max_idx -= 1
>>> kcv_errors(out['kcv_err_ts'][:tau_max_idx,:],
...            np.log10(tau_range[:tau_max_idx]), np.log10(lambda_range),
...            r'$log_{10}(\tau)$', r'$log_{10}(\lambda)$')
>>> plt.show()
```



The (almost completely) nested list of relevant variables is stored in the `selected_list` entry of the resulting `dict` object:

```
>>> for mu, sel in zip(mu_range, out['selected_list']):
...     print "%.3f:" % mu, sel.nonzero()[0]
0.000: [ 3  4  5 10 12 14]
0.001: [ 1  2  3  4  5  6  7  8  9 10 11 12 13 14]
0.010: [ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14]
0.100: [ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14]
1.000: [ 0  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 22 24 29 32 35 38 39]
```

Remembering that in the used dataset we have *3* groups of *5* relevant variables, with indexes from *0* to *14*, the result shows that the minimal list contains two variables belonging to the first group (indexes *3* and *4*), one variable belonging to the second group (index *5*) and three variables belonging to the third group (indexes *10, 12* and *14*), without any noisy variables! Incrementing the correlation parameter all the relevant variables can be included obtaining a model with (almost) constant prediction power.

In fact, the test error evaluated by the *RLS* solution computed on the selected variables (with the optimal value of λ) is:

```
>>> for mu, err in zip(mu_range, out['err_ts_list']):
...     print "%.3f: %.3f" % (mu, err)
0.000: 2.131
0.001: 2.236
0.010: 2.224
0.100: 2.224
1.000: 2.227
```

1.2.6 Appendix: functions used in this tutorial

`plot.`**`kcv_errors`**(*errors*, *range_x*, *range_y*, *label_x*, *label_y*)

Plot a 3D error surface.

Parameters

errors : (N, D) ndarray

Error matrix.

range_x : array_like of N values

First axis values.

range_y : array_like of D values

Second axis values.

label_x : str

First axis label.

label_y : str

Second axis label.

Examples

```
>>> errors = numpy.empty((20, 10))
>>> x = numpy.arange(20)
>>> y = numpy.arange(10)
>>> for i in range(20):
...     for j in range(10):
...         errors[i, j] = (x[i] * y[j])
...
>>> kcv_errors(errors, x, y, 'x', 'y')
>>> plt.show()
```

dataset_generation.**correlated_dataset**(*num_samples*, *num_variables*, *groups*, *weights*, *variables_stdev=1.0*, *correlations_stdev=0.01*, *labels_stdev=0.01*)

Random supervised dataset generation with correlated variables.

The function returns a supervised training set with `num_samples` examples with `num_variables` variables.

Parameters

num_samples : int

Number of samples.

num_variables : int

Number of variables.

groups : tuple of int

For each group of relevant variables indicates the group cardinality.

weights : array_like of sum(groups) float

True regression model.

variables_stdev : float, optional (default is *1.0*)

Standard deviation of the zero-mean Gaussian distribution generating variables column vectors.

correlations_stdev : float, optional (default is *1e-2*)

Standard deviation of the zero-mean Gaussian distribution generating errors between variables which belong to the same group

labels_stdev : float, optional (default is *1e-2*)

Standard deviation of the zero-mean Gaussian distribution generating regression errors.

Returns

X : (`num_samples`, `num_variables`) ndarray

Data matrix.

Y : (`num_samples`, 1) ndarray

Regression output.

Notes

The data will have `len(groups)` correlated groups of variables, where for each one the function generates a column vector $\mathbf{x}$ of `num_samples` values drawn from a zero-mean Gaussian distribution with standard deviation equal to `variables_stdev`.

For each variable of the group associated with the $\mathbf{x}$ vector, the function generates the values as

$$\mathbf{x}^j = \mathbf{x} + \epsilon_x,$$

where ϵ_x is additive noise drawn from a zero-mean Gaussian distribution with standard deviation equal to `correlations_stdev`.

The regression values will be generated as

$$\mathbf{Y} = \tilde{\mathbf{X}}\tilde{\boldsymbol{\beta}} + \epsilon_y,$$

where $\tilde{\boldsymbol{\beta}}$ is the `weights` parameter, a list of `sum(groups)` coefficients of the relevant variables, $\tilde{\mathbf{X}}$ is the submatrix containing only the column related to the relevant variables and ϵ_y is additive noise drawn from a zero-mean Gaussian distribution with standard deviation equal to `labels_stdev`.

At the end the function returns the matrices $\mathbf{X}$ and $\mathbf{Y}$ where

$$\mathbf{X} = [\tilde{\mathbf{X}}; \mathbf{X_N}]$$

is the concatenation of the matrix $\tilde{\mathbf{X}}$ with the relevant variables with `num_variables - sum(groups)` noisy variables generated indipendently using values drawn from a zero-mean Gaussian distribution with standard deviation equal to `variables_stdev`.

Examples

```
>>> X, Y = correlated_dataset(30, 40, (5, 5, 5), [3.0]*15)
>>> X.shape
(30, 40)
>>> Y.shape
(30, 1)
```

CHAPTER

TWO

MAIN FUNCTIONS (L1L2PY)

This module implements the two main stages of the $\ell_1\ell_2$ with double optimization variable selection, as in [DeMol09b].

Given a supervised training set $(\mathbf{X}, \mathbf{Y})$, the aim is to select a linear model built on few relevant input variables with good prediction ability.

The linear model is $\mathbf{X}\boldsymbol{\beta}$, where $\boldsymbol{\beta}$ is found as the minimizer of the (naive) elastic-net functional combined with a regularized least squares functional.

$$\frac{1}{n}\|\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \mu\|\boldsymbol{\beta}\|_2^2 + \tau\|\boldsymbol{\beta}\|_1$$

$$\frac{1}{n}\|\mathbf{Y} - \tilde{\mathbf{X}}\tilde{\boldsymbol{\beta}}\|_2^2 + \lambda\|\tilde{\boldsymbol{\beta}}\|_2^2$$

in which $\tilde{\boldsymbol{\beta}}$ and $\tilde{\mathbf{X}}$ represent, respectively, the weights vector and the input matrix restricted to the genes selected by the $\ell_1\ell_2$ selection.

The optimal solution depends on two regularization parameters, τ and λ and one correlation parameter μ and is found in two different stages:

- **Stage I** (`minimal_model`)

  This stage aims at selecting the optimal pair of regularization parameters τ_{opt} and λ_{opt} within a k-fold cross validation loop for a fixed and small value of the correlation parameter μ.

  The function follows exactly the pesudocode described in [DeMol09b] (pag.7 - Stage I).

- **Stage II** (`nested_models`)

  For fixed τ_{opt} and λ_{opt}, Stage II identifies the set of relevant lists of variables for increasing values of the correlation parameter μ.

  Note: For τ_{opt} and λ_{opt} the lists of relevant variables have same prediction power [DeMol09a].

  The function performs exactly the pesudocode described in [DeMol09b] (pag.7 - Stage II).

This module also provide a wrapper function (`model_selection`) that runs the two stages sequentially.

2.1 Stage I: Minimal Model Selection

l1l2py.**minimal_model**(*data*, *labels*, *mu*, *tau_range*, *lambda_range*, *cv_splits*, *error_function*, *data_normalizer=None*, *labels_normalizer=None*)

Minimal model selection.

Given a supervised training set (`data` and `labels`), for a fixed value of `mu` (should be minimum), it finds the values in `tau_range` and `lambda_range` minimizing the prediction error via cross validation (see error functions in the `l1l2py.tools` module).

Cross validation splits must be provided (`cv_splits`) as a list of pairs containing traning-set and validation-set indexes (see cross validation tools in the `l1l2py.tools` module).

Data and labels will be normalized on each split using the function `data_normalizer` and `labels_normalizer` (see data normalization functions in the `l1l2py.tools` module).

Warning: On each cross validation split the number of valid solutions (not void) may be different (on high values of `tau`). The function calculates the optimum value of `tau` for which the model is not void on all cross validation splits.
This means than in extreme cases the output could be void.

Parameters

data : (N, P) ndarray

Data matrix.

labels : (N,) or (N, 1) ndarray

Labels vector.

mu : float

Minimum *l2* norm penalty (*l1l2* functional).

tau_range : array_like of *T* floats

l1 norm penalties (*l1l2* functional).

lambda_range : array_like *L* of floats

l2 norm penalties (*RLS* functional).

cv_splits : array_like of tuples

Each tuple contains two lists with the training set and testing set indexes.

error_function : function object

Cross validation error function.

data_normalizer : function object, optional (default is *None*)

Data normalization function.

labels_normalizer : function object, optional (default is *None*)

Labels normalization function.

Returns

err_ts : (< T, L) ndarray

Matrix of average cross validation error on the training set. The first dimension depends on the number of valid `tau` values, **even zero**.

err_tr : (< T, L) ndarray

Matrix of average cross validation error on the training set. The first dimension depends on the number of valid `tau` values, **even zero**.

Raises

ValueError :

If the given range of `tau` values produces all void solutions with the given data splits.

2.2 Stage II: Nested lists generation

l1l2py.**nested_models**(*data*, *labels*, *test_data*, *test_labels*, *mu_range*, *tau*, *lambda_*, *error_function*, *data_normalizer=None*, *labels_normalizer=None*, *return_predictions=False*)

The function generates the models with the (almost) nested lists of selected variables.

Given a training set (`data` and `labels`) and a test set (`test_data` and `test_labels`), for fixed values of `tau` and `lambda` (should be the optimal values estimated at Stage I), it calculates one model for each increasing value in `mu_range`.

Data and labels will be normalized using the function `data_normalizer` and `labels_normalizer` (see data normalization functions in the `l1l2py.tools` module).

The function returns test and training errors using the `error_function` provided (see error functions in the `l1l2py.tools` module).

Parameters

data : (N, P) ndarray

Data matrix.

labels : (N,) or (N, 1) ndarray

Labels vector.

test_data : (T, P) ndarray

Test set matrix.

test_labels : (T,) or (T, 1) ndarray

Test set labels vector.

mu_range : array_like of M floats

l2 norm penalties (*l1l2* functional).

tau : float

Optimal *l1* norm penalty (*l1l2* functional).

lambda_: float :

Optimal *l2* norm penalty (*RLS* functional).

error_function : function object

Error function.

data_normalizer : function object, optional (default is *None*)

Data normalization function.

labels_normalizer : function object, optional (default is *None*)

Labels normalization function.

Returns

beta_list : list of M (S,1) ndarray

Models calculated for each value in `mu_range`.

selected_list : list of M (P,) ndarray of boolean

Selected feature for each models calculated.

err_ts_list : list of M floats

Test error for the models calculated.

err_tr_list : list of M floats

Training error for the models calculated.

prediction_ts_list : list of M (T, 1) ndarray

Prediction vector calculated for each value in `mu_range` on the test set.

prediction_tr_list : list of M (N, 1) ndarray

Prediction vector calculated for each value in `mu_range` on the training set.

Raises

ValueError :

If the given value of `tau` produces a void solution with the given data.

2.3 Complete model selection

`l1l2py.model_selection`(*data*, *labels*, *test_data*, *test_labels*, *mu_range*, *tau_range*, *lambda_range*, *cv_splits*, *cv_error_function*, *error_function*, *data_normalizer=None*, *labels_normalizer=None*, *sparse=False*, *regularized=True*, *return_predictions=False*)

Complete model selection procedure.

It executes the two stages implemented in `minimal_model` and `nested_models` and returns their output wrapped in a dictionary.

Note that the error function calculated in the *Stage I* may have more than one minimum.

By default the less sparse but more regularized solution (minimum value of `tau` and maximum value of `lambda`) is selected, **in the set of (tau, lambda) pairs with minimum error**, .

The boolean parameters `sparse` and `regularized` allow to change this behaviour.

Note: See the functions documentation for details on each stage and the meaning of each parameter. The **Parameters** section describes only the `sparse` and `regularized` parameters.

Parameters

sparse : bool, optional (default is *False*)

If *True*, the function selects at STAGE I the sparsest solution with minimum cross validation error.

regularized : bool, optional (default is *True*)

If *True*, the function selects at STAGE I the most regularized solution with minimum cross validation error.

Returns

out : dict

Output dictionary. According with the parameters the dictionary has the following keys:

kcv_err_ts
[(T, L) ndarray] [STAGE I] Mean cross validation errors on the training set.

kcv_err_tr
[(T, L) ndarray] [STAGE I] Mean cross validation errors on the training set.

tau_opt
[float] Optimal value of tau selected in `tau_range`.

lambda_opt
[float] Optimal value of lambda selected in `lambda_range`.

beta_list
[list of M (S,1) ndarray] [STAGE II] Models calculated for each value in `mu_range`.

selected_list
[list of M (P,) ndarray of boolean] [STAGE II] Selected variables for each model calculated.

err_ts_list
[list of M floats] [STAGE II] List of Test errors evaluated for the all the models.

err_tr_list
[list of M floats] [STAGE II] List of Training errors evaluated for the all the models.

prediction_ts_list
[list of M two-dimensional ndarray, optional] [STAGE II] Prediction vectors for the models evaluated on the test set.

prediction_tr_list
[list of M two-dimensional ndarray, optional] [STAGE II] Prediction vectors for the models evaluated on the training set.

CHAPTER

THREE

ALGORITHMS (`l1l2py.algorithms`)

In order to describe the function implemented in this module, we have to assume some notation.

Assuming to have a centered data matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$ and a column vector of regression values $\mathbf{Y} \in \mathbb{R}^n$ or binary labels $\mathbf{Y} \in \{-1, 1\}^n$, we want to minimize the regression/classification error solving a Regularized Least Square (RLS) problem.

In this module two main algorithms are implemented. The first one solves a classical RLS problem with a penalty on the ℓ_2-norm of the vector $\boldsymbol{\beta}$ (also called `ridge_regression`)

$$\boldsymbol{\beta}^* = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \left\{ \frac{1}{n} \|\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \mu \|\boldsymbol{\beta}\|_2^2 \right\}, \tag{3.1}$$

with $\mu > 0$.

The second one minimizes a functional with a linear combination of two penalties on the ℓ_1-norm and ℓ_2-norm of the vector $\boldsymbol{\beta}$ (also called `l1l2_regularization`)

$$\boldsymbol{\beta}^* = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \left\{ \frac{1}{n} \|\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \mu \|\boldsymbol{\beta}\|_2^2 + \tau \|\boldsymbol{\beta}\|_1 \right\}, \tag{3.2}$$

with $\mu > 0$ and $\tau > 0$.

3.1 Implementation details

While (3.1) has closed-form solution, for (3.2) there are many different approaches. In this module we provide an Iterative Shrinkage-Thresholding Algorithm (ISTA) proposed in [DeMol09a] exploiting a faster variation (called FISTA) proposed in [Beck09].

Starting from a null vector $\boldsymbol{\beta}$, each step updates the value of $\boldsymbol{\beta}$ until convergence:

$$\boldsymbol{\beta}^{(k+1)} = \mathbf{S}_{\frac{\tau}{\sigma}}((1 - \frac{\mu}{\sigma})\boldsymbol{\beta}^k + \frac{1}{n\sigma}\mathbf{X}^\mathbf{T}[\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}^k])$$

where, $\mathbf{S}_{\gamma>0}$ is the soft-thresholding function

$$\mathbf{S}_\gamma(x) = \text{sign}(x)\max(0, |x| - \gamma/2)$$

The constant σ is a (theorically optimal) step size which depends on the data:

$$\sigma = \frac{e}{n} + \mu,$$

where e is the maximum eigenvalue of the matrix $\mathbf{X^T X}$.

The convergence is reached when for each $j \in \{0, \ldots, d-1\}$:

$$|\beta_j^k - \beta_j^{k-1}| \leq |\beta_j^k| * (tol/k),$$

where $tol > 0$ and before k reaches a fixed maximum number of iterations.

3.2 Regularization Algorithms

l1l2py.algorithms.**ridge_regression**(*data*, *labels*, *mu=0.0*)

Implementation of the Regularized Least Squares solver.

It solves the ridge regression problem with parameter `mu` on the *l2-norm*.

Parameters

data : (N, P) ndarray

Data matrix.

labels : (N,) or (N, 1) ndarray

Labels vector.

mu : float, optional (default is *0.0*)

l2-norm penalty.

Returns

beta : (P, 1) ndarray

Ridge regression solution.

Examples

```
>>> X = numpy.array([[0.1, 1.1, 0.3], [0.2, 1.2, 1.6], [0.3, 1.3, -0.6]])
>>> beta = numpy.array([0.1, 0.1, 0.0])
>>> Y = numpy.dot(X, beta)
>>> beta = l1l2py.algorithms.ridge_regression(X, Y, 1e3).T
>>> len(numpy.flatnonzero(beta))
3
```

l1l2py.algorithms.**l1l2_regularization**(*data*, *labels*, *mu*, *tau*, *beta=None*, *kmax=100000*, *tolerance=1e-05*, *return_iterations=False*, *adaptive=False*)

Implementation of the Fast Iterative Shrinkage-Thresholding Algorithm to solve a least squares problem with *l1l2* penalty.

It solves the *l1l2* regularization problem with parameter `mu` on the *l2-norm* and parameter `tau` on the *l1-norm*.

Parameters

data : (N, P) ndarray

Data matrix.

labels : (N,) or (N, 1) ndarray

Labels vector.

mu : float

l2-norm penalty.

tau : float

l1-norm penalty.

beta : (P,) or (P, 1) ndarray, optional (default is *None*)

Starting value for the iterations. If *None*, then iterations starts from the empty model.

kmax : int, optional (default is *1e5*)

Maximum number of iterations.

tolerance : float, optional (default is *1e-5*)

Convergence tolerance.

return_iterations : bool, optional (default is *False*)

If *True*, returns the number of iterations performed. The algorithm has a predefined minimum number of iterations equal to *10*.

adaptive : bool, optional (default is *False*)

If *True*, minimization is performed calculating an adaptive step size for each iteration.

Returns

beta : (P, 1) ndarray

l1l2 solution.

k : int, optional

Number of iterations performed.

Examples

```
>>> X = numpy.array([[0.1, 1.1, 0.3], [0.2, 1.2, 1.6], [0.3, 1.3, -0.6]])
>>> beta = numpy.array([0.1, 0.1, 0.0])
>>> Y = numpy.dot(X, beta)
>>> beta = l1l2py.algorithms.l1l2_regularization(X, Y, 0.1, 0.1)
>>> len(numpy.flatnonzero(beta))
1
```

3.3 Utility Functions

`l1l2py.algorithms.`**`l1_bound`**(*data*, *labels*)

Estimation of an useful maximum bound for the *l1* penalty term.

Fixing `mu` close to *0.0* and using the maximum value calculated with this function as `tau` in the *l1l2* regularization, the solution vector contains only zero elements.

For each value of `tau` smaller than the maximum bound the solution vector contains at least one non zero element.

Parameters

data : (N, P) ndarray

Data matrix.

labels : (N,) or (N, 1) ndarray

Labels vector.

Returns

tau_max : float

Maximum `tau`.

Examples

```
>>> X = numpy.array([[0.1, 1.1, 0.3], [0.2, 1.2, 1.6], [0.3, 1.3, -0.6]])
>>> beta = numpy.array([0.1, 0.1, 0.0])
>>> Y = numpy.dot(X, beta)
>>> tau_max = l1l2py.algorithms.l1_bound(X, Y)
>>> l1l2py.algorithms.l1l2_regularization(X, Y, 0.0, tau_max).T
array([[ 0.,  0.,  0.]])
>>> beta = l1l2py.algorithms.l1l2_regularization(X, Y, 0.0, tau_max - 1e-5)
>>> len(numpy.flatnonzero(beta))
1
```

l1l2py.algorithms.**l1l2_path**(*data*, *labels*, *mu*, *tau_range*, *beta=None*, *kmax=100000*, *tolerance=1e-05*, *adaptive=False*)

Efficient solution of different *l1l2* regularization problems on increasing values of the *l1-norm* parameter.

Finds the *l1l2* regularization path for each value in `tau_range` and fixed value of `mu`.

The values in `tau_range` are used during the computation in reverse order, while the output path has the same ordering of the *tau* values.

Note: For efficency purposes, if `mu = 0.0` and the number of non-zero values is higher than *N* for a given value of tau (that means algorithm has reached the limit of allowed iterations), the following solutions (for smaller values of `tau`) are simply the least squares solutions.

Warning: The number of solutions can differ from `len(tau_range)`. The function returns only the solutions with at least one non-zero element. For values higher than *tau_max* a solution have all zero values.

Parameters

data : (N, P) ndarray

Data matrix.

labels : (N,) or (N, 1) ndarray

Labels vector.

mu : float

l2-norm penalty.

tau_range : array_like of float

l1-norm penalties in increasing order.

beta : (P,) or (P, 1) ndarray, optional (default is *None*)

Starting value of the iterations. If *None*, then iterations starts from the empty model.

kmax : int, optional (default is *1e5*)

Maximum number of iterations.

tolerance : float, optional (default is *1e-5*)

Convergence tolerance.

adaptive : bool, optional (default is *False*)

If *True*, minimization is performed calculating an adaptive step size for each iteration.

Returns

beta_path : list of (P,) or (P, 1) ndarrays

l1l2 solutions with at least one non-zero element.

Note

The acceleration method based on *warm starts*, implemented in this function, is been theoretically proved in [Hale08].

CHAPTER

FOUR

TOOLS (L1L2PY.TOOLS)

This module contains useful functions to be used in combination with the main functions of the package.

The functions included in this module are divided in four groups:

- *Range generators*
- *Data normalizers*
- *Error functions*
- *Cross Validation utilities*

4.1 Range generators

l1l2py.tools.**linear_range**(*min_value*, *max_value*, *number*)

Linear range of values between min_value and max_value.

Sequence of `number` evenly spaced values from `min_value` to `max_value`.

Parameters

min_value : float

max_value : float

number : int

Returns

range : (`number`,) ndarray

Examples

```
>>> l1l2py.tools.linear_range(min_value=0.0, max_value=10.0, number=4)
array([  0.        ,   3.33333333,   6.66666667,  10.        ])
>>> l1l2py.tools.linear_range(min_value=0.0, max_value=10.0, number=2)
array([  0.,  10.])
>>> l1l2py.tools.linear_range(min_value=0.0, max_value=10.0, number=1)
array([ 0.])
>>> l1l2py.tools.linear_range(min_value=0.0, max_value=10.0, number=0)
array([], dtype=float64)
```

l1l2py.tools.**geometric_range**(*min_value*, *max_value*, *number*)

Geometric range of values between min_value and max_value.

Sequence of `number` values from `min_value` to `max_value` generated by a geometric sequence.

Parameters

min_value : float

max_value : float

number : int

Returns

range : (number,) ndarray

Raises

ZeroDivisionError :

If `min_value` is `0.0` or `number` is `1`

Examples

```
>>> l1l2py.tools.geometric_range(min_value=0.0, max_value=10.0, number=4)
Traceback (most recent call last):
    ...
ZeroDivisionError: float division
>>> l1l2py.tools.geometric_range(min_value=0.1, max_value=10.0, number=4)
array([ 0.1       ,  0.46415888,  2.15443469, 10.        ])
>>> l1l2py.tools.geometric_range(min_value=0.1, max_value=10.0, number=2)
array([  0.1,  10. ])
>>> l1l2py.tools.geometric_range(min_value=0.1, max_value=10.0, number=1)
Traceback (most recent call last):
    ...
ZeroDivisionError: float division
>>> l1l2py.tools.geometric_range(min_value=0.1, max_value=10.0, number=0)
array([], dtype=float64)
```

Note

The geometric sequence of n elements between a and b is

$$a,\ ar^1,\ ar^2,\ \ldots,\ ar^{n-1}$$

where the ratio r is

$$r = \left(\frac{b}{a}\right)^{\frac{1}{n-1}}$$

4.2 Data normalizers

`l1l2py.tools.`**`center`**(*matrix*, *optional_matrix=None*, *return_mean=False*)

Center columns of a matrix setting each column to zero mean.

The function returns the centered `matrix` given as input. Optionally centers an `optional_matrix` with respect to the mean value evaluated for `matrix`.

Note: A one dimensional matrix is considered as a column vector.

Parameters

matrix : (N,) or (N, P) ndarray

Input matrix whose columns are to be centered.

optional_matrix : (N,) or (N, P) ndarray, optional (default is *None*)

Optional matrix whose columns are to be centered using mean of `matrix`. It must have the same number of columns as `matrix`.

return_mean : bool, optional (default is *False*)

If *True* returns mean of `matrix`.

Returns

matrix_centered : (N,) or (N, P) ndarray

Centered `matrix`.

optional_matrix_centered : (N,) or (N, P) ndarray, optional

Centered `optional_matrix` with respect to `matrix`

mean : float or (P,) ndarray, optional

Mean of `matrix` columns.

Examples

```
>>> X = numpy.array([[1, 2, 3], [4, 5, 6]])
>>> l1l2py.tools.center(X)
array([[-1.5, -1.5, -1.5],
       [ 1.5,  1.5,  1.5]])
>>> l1l2py.tools.center(X, return_mean=True)
(array([[-1.5, -1.5, -1.5],
       [ 1.5,  1.5,  1.5]]), array([ 2.5,  3.5,  4.5]))
>>> x = numpy.array([[1, 2, 3]])              # 2-dimensional matrix
>>> l1l2py.tools.center(x, return_mean=True)
(array([[ 0.,  0.,  0.]]), array([ 1.,  2.,  3.]))
>>> x = numpy.array([1, 2, 3])                # 1-dimensional matrix
>>> l1l2py.tools.center(x, return_mean=True) # centered as a (3, 1) matrix
(array([-1.,  0.,  1.]), 2.0)
>>> l1l2py.tools.center(X, X[:,:2])
Traceback (most recent call last):
    ...
ValueError: shape mismatch: objects cannot be broadcast to a single shape
```

l1l2py.tools.**standardize**(*matrix*, *optional_matrix=None*, *return_factors=False*)

Standardize columns of a matrix setting each column with zero mean and unitary standard deviation.

The function returns the standardized `matrix` given as input. Optionally it standardizes an `optional_matrix` with respect to the mean and standard deviation evaluatted for `matrix`.

Note: A one dimensional matrix is considered as a column vector.

Parameters

matrix : (N,) or (N, P) ndarray

Input matrix whose columns are to be standardized to mean *0* and standard deviation *1*.

optional_matrix : (N,) or (N, P) ndarray, optional (default is *None*)

Optional matrix whose columns are to be standardized using mean and standard deviation of `matrix`. It must have same number of columns as `matrix`.

return_factors : bool, optional (default is *False*)

If *True*, returns mean and standard deviation of `matrix`.

Returns

matrix_standardized : (N,) or (N, P) ndarray

Standardized `matrix`.

optional_matrix_standardized : (N,) or (N, P) ndarray, optional

Standardized `optional_matrix` with respect to `matrix`

mean : float or (P,) ndarray, optional

Mean of `matrix` columns.

std : float or (P,) ndarray, optional

Standard deviation of `matrix` columns.

Raises

ValueError :

If `matrix` has only one row.

Examples

```
>>> X = numpy.array([[1, 2, 3], [4, 5, 6]])
>>> l1l2py.tools.standardize(X)
array([[-0.70710678, -0.70710678, -0.70710678],
       [ 0.70710678,  0.70710678,  0.70710678]])
>>> l1l2py.tools.standardize(X, return_factors=True)
(array([[-0.70710678, -0.70710678, -0.70710678],
       [ 0.70710678,  0.70710678,  0.70710678]]), array([ 2.5,  3.5,  4.5]), array([ 2.12132
>>> x = numpy.array([[1, 2, 3]])                    # 1 row matrix
>>> l1l2py.tools.standardize(x, return_factors=True)
Traceback (most recent call last):
    ...
ValueError: 'matrix' must have more than one row
>>> x = numpy.array([1, 2, 3])                      # 1-dimensional matrix
>>> l1l2py.tools.standardize(x, return_factors=True) # standardized as a (3, 1) matrix
(array([-1.,  0.,  1.]), 2.0, 1.0)
>>> l1l2py.tools.center(X, X[:,:2])
Traceback (most recent call last):
    ...
ValueError: shape mismatch: objects cannot be broadcast to a single shape
```

4.3 Error functions

`l1l2py.tools.`**`regression_error`**(*labels*, *predictions*)

Returns regression error.

The regression error is the sum of the quadratic differences between the `labels` values and the `predictions` values, over the number of samples.

Parameters

labels : array_like, shape (N,)

Regression labels.

predictions : array_like, shape (N,)

Regression labels predicted.

Returns

error : float

Regression error calculated.

Note

The regression error is calculated using the formula

$$error = \frac{\sum_{i=1}^{N} |l_i - p_i|^2}{N} \qquad l_i \in labels, p_i \in predicted$$

`l1l2py.tools.`**`classification_error`**(*labels*, *predictions*)

Evaluate the binary classification error.

The classification error is based on the sign of the `predictions` values, with respect to the sign of the data `labels`.

The function assumes that `labels` contains positive values for one class and negative values for the other one.

Warning: For efficiency reasons, the values in `labels` are not checked by the function.

Parameters

labels : array_like, shape (N,)

Classification labels (usually contains only 1s and -1s).

predictions : array_like, shape (N,)

Classification labels predicted.

Returns

error : float

Classification error evaluated.

Examples

```
>>> l1l2py.tools.classification_error(labels=[1, 1, 1], predictions=[1, 1, 1])
0.0
>>> l1l2py.tools.classification_error(labels=[1, 1, 1], predictions=[1, 1, -1])
0.3333333333333331
>>> l1l2py.tools.classification_error(labels=[1, 1, 1], predictions=[1, -1, -1])
0.6666666666666663
>>> l1l2py.tools.classification_error(labels=[1, 1, 1], predictions=[-1, -1, -1])
1.0
>>> l1l2py.tools.classification_error(labels=[1, 1, 1], predictions=[10, -2, -3])
0.6666666666666663
```

Note

The classification error is calculated using this formula

$$error = \frac{\sum_{i=1}^{N} f(l_i, p_i)}{N} \qquad l_i \in labels,\ p_i \in predictions,$$

where

$$f(l_i, p_i) = \begin{cases} 1 & \text{if } sign(l_i) \neq sign(p_i) \\ 0 & \text{otherwise} \end{cases}$$

Warning: The classification error is calculated using the `numpy.sign` function. Keep in mind that the `sign(x)` returns `0 if x==0`.

`l1l2py.tools.`**`balanced_classification_error`**(*labels*, *predictions*, *error_weights=None*)

Returns the binary classification error balanced across the size of classes.

This function returns a balanced classification error. With the default value for `error_weights`, the function assigns greater weight to the errors belonging to the smaller class.

Parameters

labels : array_like, shape (N,)

Classification labels (usually contains only 1s and -1s).

predictions : array_like, shape (N,)

Classification labels predicted.

error_weights : array_line, shape (N,), optional (default is None)

Classification error weigths. If *None* the default weights are calculated removing from each value in `labels` their mean value.

Returns

error : float

Classification error calculated.

Examples

```
>>> l1l2py.tools.balanced_classification_error(labels=[1, 1, 1], predictions=[-1, -1, -1])
0.0
>>> l1l2py.tools.balanced_classification_error(labels=[-1, 1, 1], predictions=[-1, 1, 1])
0.0
>>> l1l2py.tools.balanced_classification_error(labels=[-1, 1, 1], predictions=[1, -1, -1])
0.8888888888888895
>>> l1l2py.tools.balanced_classification_error(labels=[-1, 1, 1], predictions=[1, 1, 1])
0.4444444444444442
>>> l1l2py.tools.balanced_classification_error(labels=[-1, 1, 1], predictions=[-1, 1, -1])
0.2222222222222224
>>> l1l2py.tools.balanced_classification_error(labels=[-1, 1, 1], predictions=[-1, 1, -1],
...                                            error_weights=[1, 1, 1])
0.3333333333333331
```

Note

The balanced classification error is calculated using this formula:

$$error = \frac{\sum_{i=1}^{N} w_i \cdot f(l_i, p_i)}{N} \qquad l_i \in labels,\ p_i \in predictions,$$

where $f(l_i, p_i)$ is as defined above.

With the default weigths the error function becomes:

$$error = \frac{\sum_{i=1}^{N} |l_i - \overline{labels}| \cdot f(l_i, p_i)}{N} \qquad l_i \in labels,\ p_i \in predicted$$

Warning: If `labels` contains only values belonging to **one** class, the functions returns always *0.0* because $l_i - \overline{labels} = 0$, than $w_i = 0$ for each i.

4.4 Cross Validation utilities

`l1l2py.tools.`**`kfold_splits`**(*labels*, *k*, *rseed=0*)

k-fold cross validation splits.

Given a list of labels, the function produces a list of `k` splits. Each split is a pair of tuples containing the indexes of the training set and the indexes of the test set.

Parameters

labels : array_like, shape (N,)

Data labels.

k : int, greater than *0*

Number of splits.

rseed : int, optional (default is *0*)

Random seed.

Returns

splits : list of `k` tuples

Each tuple contains two lists with the training set and test set indexes.

Raises

ValueError :

If `k` is less than 2 or greater than *N*.

Examples

```
>>> labels = range(10)
>>> l1l2py.tools.kfold_splits(labels, 2)
[([7, 1, 3, 6, 8], [9, 4, 0, 5, 2]), ([9, 4, 0, 5, 2], [7, 1, 3, 6, 8])]
>>> l1l2py.tools.kfold_splits(labels, 1)
Traceback (most recent call last):
    ...
ValueError: 'k' must be greater than one and smaller or equal than the number of samples
```

`l1l2py.tools.`**`stratified_kfold_splits`**(*labels*, *k*, *rseed=0*)

Sstratified k-fold cross validation splits.

This function is a variation of `kfold_splits`, which returns stratified splits. The divisions are made by preserving the percentage of samples for each class, assuming that the problem is binary.

Parameters

labels : array_like, shape (N,)

Data labels (usually contains only 1s and -1s).

k : int, greater than *0*

Number of splits.

rseed : int, optional (default is *0*)

Random seed.

Returns

splits : list of `k` tuples

Each tuple contains two lists with the training set and test set indexes.

Raises

ValueError :

If *labels* contains more than two classes labels.

ValueError :

If `k` is less than 2 or greater than number of positive or negative samples in *labels*.

Examples

```
>>> labels = range(10)
>>> l1l2py.tools.stratified_kfold_splits(labels, 2)
Traceback (most recent call last):
    ...
ValueError: 'labels' must contains only two class labels
>>> labels = [1, 1, 1, 1, 1, 1, -1, -1, -1, -1]
>>> l1l2py.tools.stratified_kfold_splits(labels, 2)
[([8, 9, 5, 2, 1], [7, 6, 3, 0, 4]), ([7, 6, 3, 0, 4], [8, 9, 5, 2, 1])]
>>> l1l2py.tools.stratified_kfold_splits(labels, 1)
Traceback (most recent call last):
    ...
ValueError: 'k' must be greater than one and smaller or equal than number of positive and neg
```

Note

Running this functions more times with the same value of the parameter `rseed` gives **always** the same result, in order to allow repeatable experiments. Note, moreover, that each of this functions sets the random seed equal to `None`, to restore a random seed for the following use of the `random` module (see `random.seed`).

genindex

References

BIBLIOGRAPHY

[Hale08] E. T. Hale, W. Yin, Y. Zhang "Fixed-point continuation for ℓ_1-minimization: Methodology and convergence" SIAM J. Optim. Volume 19, Issue 3, pp. 1107-1130, 2008

[Zou05] H. Zou, T. Hastie, "Regularization and variable selection via the elastic net" J.R. Statist. Soc. B, 67 (2) pp. 301-320, 2005

[DeMol09a] C. De Mol, E. De Vito, L. Rosasco, "Elastic-net regularization in learning theory" Journal of Complexity, n. 2, vol. 25, pp. 201-230, 2009.

[DeMol09b] C. De Mol, S. Mosci, M. Traskine, A. Verri, "A Regularized Method for Selecting Nested Group of Genes from Microarray Data" Journal of Computational Biology, vol. 16, pp. 677-690, 2009.

[Beck09] A. Beck, M. Teboulle, "A fast iterative shrinkage-thresholding algorithm for linear inverse problems" SIAM Journal on Imaging Sciences, 2(1):183–202, Mar 2009.

INDEX