Package ‘COSNet’

April 25, 2017

Type Package

Title Cost Sensitive Network for node label prediction on graphs with highly unbalanced labelings

Version 1.10.0

Date 2015-11-06

Author Marco Frasca and Giorgio Valentini -- Universita’ degli Studi di Milano

Maintainer Marco Frasca <frasca@di.unimi.it>

Description Package that implements the COSNet classification algorithm. The algorithm predicts node labels in partially labeled graphs where few positives are available for the class being predicted.

License GPL (>= 2)

URL https://github.com/m1frasca/COSNet_GitHub

LazyLoad yes

Suggests bionetdata, PerfMeas, RUnit, BiocGenerics

biocViews GraphAndNetwork, Classification,Network, NeuralNetwork

NeedsCompilation yes

R topics documented:

COSNet-package ............................................ 2
COSNet .................................................. 2
cosnet.cross.validation ................................. 4
find.division.not.strat .................................. 6
find.division.strat ...................................... 6
generate_labels ........................................ 7
generate_points ....................................... 8
optimize ............................................... 9
optimize_pos_above .................................. 10
reg_data ............................................. 12
runSubnet .......................................... 13

Index 15
COSNet-package

R package for binary classification and node ranking on partially labeled graphs with unbalanced labels.

Description

Algorithm based on cost-sensitive neural network for predicting node labels in a semi-supervised setting.

Details

<table>
<thead>
<tr>
<th>Package</th>
<th>COSNet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type:</td>
<td>Package</td>
</tr>
<tr>
<td>Version:</td>
<td>1.5.1</td>
</tr>
<tr>
<td>Date:</td>
<td>2015-11-06</td>
</tr>
<tr>
<td>License:</td>
<td>GPL (&gt;= 2)</td>
</tr>
<tr>
<td>LazyLoad:</td>
<td>yes</td>
</tr>
</tbody>
</table>

This package implements the COSNet algorithm (Frasca et al. 2013). COSNet is a semi-supervised cost-sensitive neural network for predicting node labels in partially labeled graphs. The algorithm is able in inferring a labeling for unlabeled nodes in the graph starting from the graph topology and the known labels.

Author(s)

Marco Frasca, and Giorgio Valentini
DI, Dipartimento di Informatica
Università degli Studi di Milano
<{frasca,valentini}@di.unimi.it>
Maintainer: Marco Frasca

References

**COSNet**

**Description**

This function realizes the COSNet algorithm (Frasca et al. 2013). COSNet is a semi-supervised algorithm based on parametric Hopfield networks for predicting labels for unlabeled nodes in graphs which are only partially labeled.

**Usage**

\[
\text{COSNet}(W, \text{labeling}, \text{cost} = 0)
\]

**Arguments**

- \(W\): square symmetric named matrix, whose components are in the interval \([0,1]\). The \(i,j\)-th component is a similarity index between node \(i\) and node \(j\). The components of the diagonal of \(W\) are zero. Rows and columns should be named identically.
- \(\text{labeling}\): vector of node labels: 1 for positive examples, -1 for negative examples, 0 for unlabeled nodes.
- \(\text{cost}\): real value corresponding to beta parameter in the equation \(\eta = \beta \tan((\alpha - \pi/4)2)\), where \(\eta\) is the coefficient of the regularization term in the energy function (Frasca et al. 2013). If \(\text{cost} = 0\) (default) the unregularized version is executed. "cost" is a real value that reduces or increases the influence of regularization on the network dynamics. The higher the value of cost, the more the influence of the regularization term. It is suggested using small values for this parameter (e.g. \(\text{cost} = 0.0001\)).

**Details**

COSNet constructs a Hopfield network whose connection matrix is \(W\), and it applies a cost-sensitive strategy to determine the network parameters starting from \(W\) and labels "labeling". COSNet distinguishes between labeled (1, -1 components in "labeling") and unlabeled (zero components in "labeling") nodes, and it is made up by three steps: 1) Generating a random labeling (1, -1) for unlabeled nodes. 2) Learning the parameters \(\alpha\) and \(\beta\) such that the line \(\cos(\alpha)y - \sin(\alpha)x - q\cos(\alpha) = 0\" linearly separates a suitable set of labeled points (in which each point corresponds to a labeled node) and optimizes (in terms of alpha and \(q\)) the \(F\)-score criterion. The output of this phase is the intercept "\(q\)" of the optimum line and the corresponding angle "\(\alpha\)". Then each neuron has threshold \(c = - q\cos(\alpha)\). 3) Extending \(\alpha\) and \(\beta\) to the subnetwork composed of only unlabeled nodes, and simulating it until an equilibrium state is reached. The dynamics of this network is regularized by adding a term to the energy function that is minimized when the proportion of positive in the network state is roughly the proportion of positives in the labeled part of the network. The parameter "cost" corresponds to the parameter beta in the equation \(\eta = \beta \tan((\alpha - \pi/4)2)\) (see Frasca et al. 2013). When the equilibrium state is reached, positive nodes will be predicted as positive for the current task.

**Value**

COSNet returns a list with six elements:

- \(\alpha\): the optimum angle
- \(c\): the optimum threshold
- \(F\text{score}\): the optimum F-score computed in Step 2
- \(\text{pred}\): the vector of predictions for unlabeled nodes
scores: the vector of scores for unlabeled nodes
iter: number of iterations until convergence in Step 3

References


Examples

```r
library(bionetdata);
## loading Binary protein-protein interactions from the STRING database (von Mering et al. 2002)
data(Yeast.STRING.data) # "Yeast.STRING.data"
## FunCat classes annotations (0/1) for the genes included in Yeast.STRING.data. Annotations refer to the funcat-2.1 scheme, and funcat-2.1 data 20070316 data, available from the MIPS website.
data(Yeast.STRING.FunCat) # "Yeast.STRING.FunCat"
labels <- Yeast.STRING.FunCat;
labels[labels == 0] <- -1;
## excluding the dummy "00" root
labels <- labels[, -which(colnames(labels) == "00")];
n <- nrow(labels);
k <- floor(n/10);
cat("k = ", k, "\n");
## choosing the first class
labeling <- labels[, 1];
## randomly choosing a subset of genes whose labels are hidden
hidden <- sort(sample(1:n, k));
hidden.labels <- labeling[hidden];
labeling[hidden] <- 0;
out <- COSNet(Yeast.STRING.data, labeling, 0);
prediction <- out$pred;
TP <- sum(hidden.labels == 1 & prediction == 1);
FN <- sum(hidden.labels == 1 & prediction == -1);
FP <- sum(hidden.labels == -1 & prediction == 1);
out2 <- COSNet(Yeast.STRING.data, labeling, 0.0001);
prediction <- out2$pred;
TP2 <- sum(hidden.labels == 1 & prediction == 1);
FN2 <- sum(hidden.labels == 1 & prediction == -1);
FP2 <- sum(hidden.labels == -1 & prediction == 1);
```

**cosnet.cross.validation**

Cross validation procedure for the COSNet algorithm

**Description**

This function applies the function COSNet to the input data with a cross validation procedure.

**Usage**

cosnet.cross.validation(labels, W, nfolds, cost)
cosnet.cross.validation

Arguments

labels

named matrix of node labels. The (i-j)-th component contains the label (1 for positive examples, -1 for negative examples) of node i for j-th functional class to be predicted.

W

square symmetric named matrix. The (i,j)-th component is a similarity index between node i and node j. The components of the diagonal of W are zero.

nfolds

integer corresponding to the number of desired folds.

cost

real value that corresponds to the cost parameter of COSNet.

Details

cosnet.cross.validation runs the function COSNet on the input data through a cross validation procedure. For each class to be predicted (column of "labels"), both "W" and "labels" are partitioned into "nfolds" subsets and at each iteration the labels of a fold are hidden and predicted with function COSNet. When possible, input data are partitioned by ensuring the same proportion of positive and negative instances in each fold.

Value

List with three elements:

labels

1/-1 named input label matrix, in which rows correspond to nodes and columns to classes.

predictions

named 1/-1 prediction matrix, in which rows correspond to nodes and columns to classes. The position i-j-th is 1 if the node i has been predicted as positive for the class j. -1 otherwise.

scores
	named real score matrix, in which rows correspond to nodes and columns to classes. The position i-j-th is a real number corresponding to the internal energy at equilibrium for node i when predicting class j. This score is a "degree" of membership of node i to the class j.

See Also

COSNet

Examples

library(bionetdata);
data(Yeast.STRING.data)
data(Yeast.STRING.FunCat) # "Yeast.STRING.FunCat"
## excluding the dummy "00" root
Yeast.STRING.FunCat <-
    Yeast.STRING.FunCat[, -which(colnames(Yeast.STRING.FunCat) == "00")];
nfolds <- 5;
res <- cosnet.cross.validation(Yeast.STRING.FunCat[, 1:50], Yeast.STRING.data,
    nfolds, 0.0001);
## computing performances
library(PerfMeas);
perf <- F.measure.single.over.classes(res$labels, res$predictions);
cat(perf$average);
Description

Function to determine a random partition of the input vector into a specified number of folds.

Usage

find.division.not.strat(vett, n_fold)

Arguments

vett  vector to be partitioned
n_fold  number of folds in which the argument vett must be partitioned

Value

List with n_fold elements, the i-th element is a vector corresponding to i-th fold.

See Also

find.division.strat

Examples

n <- 100;
vett <- runif(n, 0, 1);
n_fold <- 5;
fold_list <- find.division.not.strat(vett, n_fold);
length(fold_list);
## indices of the first fold
fold_list[[1]];

Description

Function to determine a random partition of the labeled input vector into a fixed number of folds, such that each fold has around the same proportion of two-class labels.

Usage

find.division.strat(labels, vett, n_fold)
Arguments

labels | binary -1/1 label vector. labels[i] is the label for the element vett[i].
vett    | vector to be partitioned
n_fold  | number of folds in which the argument vett must be partitioned

Details

The input vector "vett" is randomly partitioned into "n_fold" folds ensuring each fold contains roughly the same proportions of positives and negative labels, according to the labeling "labels"

Value

List with n_fold elements, the i-th element is a vector corresponding to i-th fold.

See Also

find.division.not.strat

Examples

```r
n <- 100;
vett <- runif(n, 0, 1)
labels <- c(rep(1, floor(n/3)), rep(-1, ceiling(2*n/3)));
n_fold <- 5;
fold_list <- find.division.strat(labels, vett, n_fold);
length(fold_list);
## number of positives in the first fold
sum(labels(fold_list[1]) > 0);
```

---

generate_labels | Generate random labels

Description

Function to generate a vector of random labels

Usage

generate_labels(n, pos_rate)

Arguments

n        | number of labels to be generated
pos_rate | rate of expected positive labels

Details

This function generates "n" random labels in -1, 1 drawn from the binomial distribution B(n, pos_rate)
Value
-1/1 vector of length "n" containing the generated labels

See Also
generate_points

Examples
pos_rate <- 0.3;
n <- 100;
## generating n random labels with 0.3 expected rate of positive labels
random_labels <- generate_labels(n, pos_rate);
sum(random_labels > 0);

Description
This function associates each labeled node with a point in the plane, whose coordinates are respectively the weighted sum of its positive and negative neighborhoods

Usage
generate_points(W, unlabeled, labeling)

Arguments
W
square symmetric named matrix, whose components are in the [0,1] interval. The i,j-th component is the weight between node i and node j. The components of the diagonal of W are zero.

unlabeled
vector of the indices of the unlabeled nodes

labeling
vector of node labels: 1 for positive nodes, -1 for negative nodes, 0 for unlabeled nodes

Details
For each labeled node k, a point (pos_vect[k], neg_vect[k]) is computed, where pos_vect[k] is the weighted sum of the positive neighbors of node k and neg_vect[k] is the weighted sum of negative neighbors of node k.

Value
List of two elements:

pos_vect
is the vector of the abscissae; pos_vect[k] contains the weighted sum of the positive neighbors of node k

neg_vect
is the vector of the ordinates; neg_vect[k] contains the weighted sum of the negative neighbors of node k
References

Examples

```r
## randomly generating labels
labels <- generate_labels(100, 0.3);
unlabeled <- sample(1:100, 10);
labels[unlabeled] <- 0;
## randomly generating connection matrix
W <- matrix(sample(1:10000, 100*100)/1000, nrow = 100);
diag(W) <- 0;
points <- generate_points(W, unlabeled, labels);
points$pos_vect[1:5];
points$neg_vect[1:5];
```

---

**optimizep**

*Optimizing algorithm parameters*

**Description**

Function to learn the parameters "alpha", determining neurons activation values, and the neuron threshold "c".

**Usage**

```r
optimizep(pos_vect, neg_vect, training_labels)
```

**Arguments**

- `pos_vect`: vector of abscissae of the points to be separated
- `neg_vect`: vector of ordinates of the points to be separated
- `training_labels`: 1/-1 vector of point labels

**Details**

This function computes the optimal angle "alpha" and the optimal threshold "c". For each labeled neuron k, a point (pos_vect[k], neg_vect[k]) is considered. Points are labeled according to the labels contained in the vector "training_labels". Then the straight line, among those with positive slope, which separates these points by maximizing the F-score is learned. The line is represented by the angle alpha formed with the "x" axis, and its intercept "q" with "y" axis. When separating points by a straight line, there are two possibility: 1) Considering as positive the half-plane above the line; 2) Considering as positive the half-plane below the line. The procedure investigates both these possibilities, and also returns which choice between 1) and 2) corresponds to the best F-score.
Value

list "res" with 4 components:

- res$alpha : value of the optimum angle alpha
- res$c : value of the optimum threshold c
- res$Fscore : value of the optimum F-score
- res$pos_half : the position of the positive half-plane : > 0 in case 1), < 0 in case 2)

See Also

optimize_pos_above

Examples

```r
library(bionetdata);
data(Yeast.STRING.data);
data(Yeast.STRING.FunCat);
n <- nrow(Yeast.STRING.data);
## removing dummy node 00
Yeast.STRING.FunCat <- Yeast.STRING.FunCat[, -which(colnames(Yeast.STRING.FunCat) == "00")];
## selecting the class with index 1
class <- 1;
labels <- as.vector(Yeast.STRING.data[, class]);
names(labels) <- rownames(Yeast.STRING.FunCat);
labels <- as.vector(Yeast.STRING.FunCat[, class]);
names(labels) <- rownames(Yeast.STRING.FunCat);
## partitioning the data
folds <- find.division.strat(labels, 1:n, 3);
labels[labels <= 0] <- -1;
test.set <- folds[[1]];
training.set <- setdiff(1:n, test.set);
labels[test.set] <- 0;
## generating the points to be separated
points <- generate_points(Yeast.STRING.data, test.set, labels);
opt_parameters <- optimizep(points$pos_vect[training.set],
                           points$neg_vect[training.set], labels[training.set]);
str(opt_parameters);
```

optimize_pos_above  Alternative algorithm for optimizing parameters

Description

Alternative algorithm to compute the two parameters: 'alpha', determining neurons activation values, and the neuron thresholds 'c'.

Usage

```r
optimize_pos_above(pos_vect, neg_vect, training_labels, res)
```
**optimize_pos_above**

**Arguments**

- `pos_vect`: vector of abscissae of the points to be separated
- `neg_vect`: vector of ordinates of the points to be separated
- `training_labels`: 1/-1 vector of the point labels
- `res`: list containing the optimum angle (field `alpha`), neuron threshold (field `c`), maximum F-score (field `Fscore`) and positive halfplane (field `pos_half`) computed by the procedure corresponding to the choice 1) of function `optimizep`.

**Details**

Function to optimize the the parameters 'alpha' and 'c' when the function `optimizep` determines that the maximum F-score corresponds to the half-plane above the separation line. The algorithm works in three steps: 1) Selecting all the points which lie on the Y-axis. The aim is to choose a positive point which will be the center of the line bundle we consider in the next step. We sort the selected points by ordinate and for each positive point we compute the F-score of the almost vertical line (but with negative slope) crossing this point considering solely the selected points. Then we choose the point k which corresponds to the highest F-score. 2) The algorithm computes the slopes of the lines crossing the point k and each point not lying on the Y-axis. Then it searches the line, among those with negative slope, which maximizes the F-score criterion by sorting the computed lines according to their slopes in an increasing order. Consequently, the angle alpha relative to the optimum line is in the interval $[\pi/2, \pi[$. 3) Compute the intercepts of the straight lines whose slope is $\tan(\alpha)$ and crossing each available point. The optimum line is identified by scanning the computed lines according to their intercept in an increasing order. Let q be the intercept of the optimum line $y = \tan(\alpha)z + q$, then we set $c = -\cos(\alpha)q$. If there are no positive point with abscissa 0, the function returns the optimal parameters contained in input argument 'res' computed by the procedure corresponding to the choice 1) of function `optimizep`.

**Value**

list res with 3 components

- `res$alpha`: value of the optimum angle alpha
- `res$c`: value of the optimum threshold c
- `res$Fscore`: value of the optimum F-score
- `res$pos_half`: position of the positive half-plane (-1 below, 1 above the optimum straight line)

**See Also**

- `optimizep`

**Examples**

```r
library(bionetdata);
data(Yeast.STRING.data);
data(Yeast.STRING.FunCat);
n <- nrow(Yeast.STRING.data);
## removing dummy node 0
Yeast.STRING.FunCat <- Yeast.STRING.FunCat[, -which(colnames(Yeast.STRING.FunCat) == "0")];
## selecting the class with index 1
class <- 1;
```
labels <- as.vector(Yeast.STRING.data[, class]);
names(labels) <- rownames(Yeast.STRING.FunCat);
labels <- as.vector(Yeast.STRING.FunCat[, class]);
names(labels) <- rownames(Yeast.STRING.FunCat);
## partitioning the data
folds <- find.division.strat(labels, 1:n, 3);
labels[labels <= 0] <- -1;
test.set <- folds[[1]];
training.set <- setdiff(1:n, test.set);
labels[test.set] <- 0;
points <- generate_points(Yeast.STRING.data, test.set, labels);
## setting values for the parameter
res <- list(alpha=pi/2, c=0, Fscore=0, pos_half=-1);
opt_parameters <- optimize_pos_above(points$pos_vect[training.set],
points$neg_vect[training.set], labels[training.set], res);
str(opt_parameters);

reg_data

Function to compute the regularized version of COSNet (Frasca et al. 2013)

Description

This function modifies the weights and the thresholds of the network to realize the COSNet regularization.

Usage

reg_data(W, theta, eta, M, m, pos_num)

Arguments

W  square symmetric named matrix of the network weights. The components of W are in the [0,1] interval. The i,j-th component is the weight between neuron i and neuron j. The components of the diagonal of W are 0
theta  vector of the neuron activation thresholds
eta  real value corresponding to the eta regularization coefficient in the energy function (Frasca et al. 2013). If eta = 0 no regularization is applied. The higher the value of eta, the more the influence of the regularization term
M  positive neuron activation value
m  negative neuron activation value
pos_num  number of expected positive neurons in the equilibrium state of the network

Value

list of two element:
W  the regularized connection matrix
theta  regularized threshold vector
References


Examples

```r
library(bionetdata);
data(Yeast.STRING.data);
n <- nrow(Yeast.STRING.data);
dim(Yeast.STRING.data);
range(Yeast.STRING.data);
## setting values for parameter alpha, for the rate of positive examples,
## for neuron thresholds and for eta parameter
alpha <- 1;
pos.rate <- 0.01;
thresholds <- runif(n);
range(thresholds);
eta <- 0.001;
a <- reg_data(Yeast.STRING.data, thresholds, eta, sin(alpha),
               -cos(alpha), ceiling(pos.rate*n));
## new connection matrix
dim(a$W);
range(a$W);
## new thresholds
range(a$theta);
```

---

runSubnet  

Realizing the network dynamics.

Description

Function to simulate the dynamics of the network composed of unlabeled nodes.

Usage

```r
runSubnet(W, labeling, alpha_value, c_value, cost)
```

Arguments

- **W**: square symmetric named matrix, whose components are in the interval [0,1]. The i,j-th component is a similarity index between node i and node j. The components of the diagonal of W are zero. Rows and columns should be named identically.
- **labeling**: vector of node labels: 1 for positive examples, -1 for negative examples, 0 for unlabeled nodes
- **alpha_value**: real value in [0, pi/2], determining the neuron activation values: sin(alpha) and -cos(alpha).
- **c_value**: real value used as activation threshold for each neuron
cost real value corresponding to beta parameter in the equation \( \eta = \beta \tan((\alpha - \pi/4)^2) \), where \( \eta \) is the coefficient of the regularization term in the energy function (Frasca et al. 2013). If \( \text{cost} = 0 \) (default) the unregularized version is executed. The higher the value of \( \text{cost} \), the more the influence of the regularization term. It is suggested using small values for this parameter (e.g. \( \text{cost} = 0.00001 \)).

Details

Function to simulate the subnetwork composed of the unlabeled genes, in which each neuron has \( \sin(\text{alpha}_\text{value}), -\cos(\text{alpha}_\text{value}) \) as activation value, and in which each neuron has a threshold "c_value" minus the contribution from the labeled neighbors.

Value

list with three components:

- **state** Named vector of prediction (at equilibrium) for unlabeled nodes
- **scores** Named vector of scores (at equilibrium) for unlabeled nodes
- **iter** Number of iterations of the network until convergence

References


Examples

```r
library(bionetdata);
data(Yeast.STRING.data);
data(Yeast.STRING.FunCat);
n<-nrow(Yeast.STRING.data);
## removing dummy node 00
Yeast.STRING.FunCat <- Yeast.STRING.FunCat[, -which(colnames(Yeast.STRING.FunCat) == "00")];
class <- 1;
labels <- as.vector(Yeast.STRING.data[, class]);
names(labels) <- rownames(Yeast.STRING.FunCat);
labels <- as.vector(Yeast.STRING.FunCat[, class]);
names(labels) <- rownames(Yeast.STRING.FunCat);
folds <- find.division.strat(labels, 1:n, 3);
labels[labels <= 0] <- -1;
test.set <- folds[[1]];
training.set <- setdiff(1:n, test.set);
labels[test.set] <- 0;
res <- runSubnet(Yeast.STRING.data, labels, alpha=1, c=0, cost=0.0001);
str(res);
```
Index

*Topic** package
  COSNet-package, 2

COSNet, 2, 5
COSNet-package, 2
cosnet.cross.validation, 4

find.division.not.strat, 6, 7
find.division.strat, 6, 6

generate_labels, 7
generate_points, 8

optimize_pos_above, 10, 10
optimizep, 9, 11

reg_data, 12
runSubnet, 13