Package 'PReMiuM'

January 10, 2013

| Package | |
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| Post processing for C++ PReMiuM | |
| n 3.0.4 | |
| 2012-19-12 | |
| | |
| ainer Silvia Liverani <liveranis@gmail.com></liveranis@gmail.com> | |
| ption Dirichlet process Bayesian Clustering, also known as profile regression. | |
| e GPL (>= 3) | |
| oad yes | |
| | |
| gTo Rcpp | |
| nRequirements GNU make | |
| pics documented: | |
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Description

Dirichlet Process Bayesian Clustering and functions for the post-processing of its output.

Details

Package: PReMiuM Type: Package Version: 3.0.1 Date: 2012-12-19

License: What license is it under?

LazyLoad: yes

~~ An overview of how to use the package, including the most important ~~ ~~ functions ~~

Author(s)

David Hastie and Silvia Liverani

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References

Hastie et al (2012) blah blah

calcAvgRiskAndProfile 3

```
riskProfileObj<-calcAvgRiskAndProfile(clusObj)
clusterOrderObj<-plotRiskProfile(riskProfileObj, "summary.png")</pre>
```

calcAvgRiskAndProfile Calculation of the average risks and profiles

Description

Calculation of the average risks and profiles.

Usage

```
calcAvgRiskAndProfile(clusObj, includeFixedEffects=F)
```

Arguments

```
clusObj Object of type clusObj.
includeFixedEffects
By default this is set to 'FALSE'.
```

Value

Need to write this

none dont know

Author(s)

David Hastie and Silvia Liverani

```
generateDataList <- clusSummaryBernoulliDiscrete()
inputs <- generateSampleDataFile(generateDataList)
runInfoObj<-profRegr(yModel=inputs$yModel, xModel=inputs$xModel, nSweeps=100,
    nBurn=100, data=inputs$inputData, output="output",
    covNames=inputs$covNames)

dissimObj<-calcDissimilarityMatrix(runInfoObj)
clusObj<-calcOptimalClustering(dissimObj)
riskProfileObj<-calcAvgRiskAndProfile(clusObj)
clusterOrderObj<-plotRiskProfile(riskProfileObj,"summary.png",
    whichCovariates=c(1,2))</pre>
```

calcDissimilarityMatrix

Calculates the dissimilarity matrix

Description

Calculates the dissimilarity matrix.

Usage

```
calcDissimilarityMatrix(runInfoObj)
```

Arguments

runInfo0bj Object of type runInfoObj.

Value

Need to write this

disSimRunInfoObj

These are details regarding the run and in the same format as runInfoObj.

disSimMat The dissimilarity matrix, in vector format. Note that it is diagonal, so this con-

tains the upper triangle diagonal entries.

disSimMatPred The dissimilarity matrix, again in vector format as above, for the predicted sub-

jects.

1sOptSweep The optimal partition among those explored by the MCMC, as defined by the

least squares method. See Dahl (2006).

Author(s)

David Hastie and Silvia Liverani

calcOptimalClustering 5

calcOptimalClustering Calculation of the optimal clustering

Description

Calculates the optimal clustering.

Usage

calcOptimalClustering(disSimObj, maxNClusters=NULL, useLS=F)

Arguments

disSimObj A dissimilarity matrix (in vector format, as the output of the function calcDis-

similarityMatrix(), and as described in ?calcDissimilarityMatrix) or a list of dis-

similarity matrix, to combine the output of several runs of the MCMC.

maxNClusters Set the maximum number of clusters allowed. This is set to the maximum num-

ber explored.

useLS This is set to FALSE by default. If it is set to TRUE then the least-squares

method is used for the calculation of the optimal clustering, as described in

Molitor et al (2010).

Value

the output is a list with the following elements.

clusObjRunInfoObj

Details on this run.

clusterSizes Cluster sizes.

clusteringPred The predicted cluster memberships for the predicted scenarios.

clusObjDisSimMat

Dissimilarity matrix.

clustering Cluster memberships.

nClusters Optimal number of clusters.

avgSilhouetteWidth

Not sure

Author(s)

David Hastie and Silvia Liverani

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Examples

calcPredictions

Calculates the predictions

Description

Calculates the predictions.

Usage

```
calcPredictions(riskProf0bj,
    predictResponseFileName=NULL,
    doRaoBlackwell=F,fullSweepPredictions=F,fullSweepLogOR=F)
```

Arguments

NOTE: THIS DESCRIPTION HAS NOT BEEN CHANGED FOR R AND THE FUNCTIONALITY HAVE NOT BEEN ADAPTED YET

There is also now an additional function calcPredictions for computing predicted responses, for various prediction scenarios. It is assumed that the predictive allocations and Rao-Blackwell predictions have already been done in C++ (using the –predict=<filename> run time option). The user can provide the function with a file through the predictResponseFileName argument. This file has the number of subjects, followed by a row for each subject, where each row contains values for the response, fixed effects and offset / number of trials (depending on the response model) where available. Missing values in this file are denoted (-999). If the file is not provided then the response, fixed effect and offset data is treated as missing for all subjects. If a subject is missing fixed effect values, then the mean value or 0 category fixed effect is used in the predictions (i.e. no fixed effect contribution to predicted response). If the offset / number of trials is missing this value is taken to be 1 when making predictions. If the response is provided for all subjects, the predicted responses are compared with the observed responses and the bias and rmse are computed.

The function can produce predicted values based on simple allocations (the default), or a Rao-Blackwellised estimate of predictions, where the probabilities of allocations are used instead of actually performing a random allocation.

calcPredictions 7

An example file where the fixed effects can be provided for prediction but the observed response is missing is data/input/example_Poisson_Normal_predictW.txt (there are 2 fixed effects in this example). An example of using the function, which would do the Rao Blackwellised predictions, is given by

>calcPredictions(riskProfileObj, predictResponseFileName='../data/input/example_Poisson_Normal_predoRaoBlackwell=T)

An example file where both the observed response and fixed effects are present is in data/input/example_Poisson_Normal_predictYW.txt (there are no fixed effects in this example, but these would just be added as columns between the first and last columns). An example of using the function, which would do the simple predictions using the allocations produced by the C++, is given by

>calcPredictions(riskProfileObj, predictResponseFileName='../data/input/example_Poisson_Normal_predoRaoBlackwell=F)

Object of type riskProfObj.

predictResponseFileName

riskProf0bj The file which contains the predictive scenarios, as it is produced by the code

and stored.

doRaoBlackwell By default this is set to FALSE.

fullSweepPredictions

By default this is set to FALSE.

fullSweepLogOR By default this is set to FALSE.

Value

Need to write this

none

it creates files outside

Author(s)

David Hastie and Silvia Liverani

```
riskProfileObj <- calcAvgRiskAndProfile(clusObj)
clusterOrderObj <- plotRiskProfile(riskProfileObj,"summary.png",
    whichCovariates=c(1,2))
output_predictions <- calcPredictions(riskProfileObj,fullSweepPredictions=TRUE)</pre>
```

clusSummaryBernoulliDiscrete

Definition of characteristics of sample datasets for profile regression

Description

.

Usage

```
clusSummaryBernoulliDiscrete()
clusSummaryBernoulliDiscrete()
clusSummaryBinomialNormal()
clusSummaryCategoricalDiscrete()
clusSummaryNormalDiscrete()
clusSummaryNormalNormal()
clusSummaryPoissonDiscrete()
clusSummaryPoissonNormal()
clusSummaryVarSelectBernoulliDiscrete()
clusSummaryBernoulliMixed()
```

Value

Need to write this

none List of stuff

Author(s)

David Hastie and Silvia Liverani

Examples

 ${\tt clusSummaryBernoulliDiscrete()}$

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compareClustering

Function to compare different partitions

Description

Function to compare different partitions.

Usage

```
compareClustering(riskProfileObjA, riskProfileObjB, clusterOrder=NULL)
```

Arguments

```
riskProfileObjA dont know
riskProfileObjB dont know
clusterOrder dont know
```

Value

Need to look into this, I don't know how it compares them.

Author(s)

David Hastie and Silvia Liverani

```
# simulate a dataset
generateDataList <- clusSummaryBernoulliDiscrete()</pre>
inputs <- generateSampleDataFile(generateDataList)</pre>
# do clustering a first time
runInfoObjA<-profRegr(yModel=inputs$yModel, xModel=inputs$xModel,</pre>
    nSweeps=100, nBurn=100, data=inputs$inputData, output="output",
    covNames=inputs$covNames)
dissimObjA<-calcDissimilarityMatrix(runInfoObjA)</pre>
clusObjA<-calcOptimalClustering(dissimObjA)</pre>
riskProfileObjA<-calcAvgRiskAndProfile(clusObjA)</pre>
# do clustering a second time
runInfoObjB<-profRegr(yModel=inputs$yModel, xModel=inputs$xModel,</pre>
    nSweeps=100, nBurn=100, data=inputs$inputData, output="output",
    covNames=inputs$covNames)
dissimObjB<-calcDissimilarityMatrix(runInfoObjB)</pre>
clusObjB<-calcOptimalClustering(dissimObjB)</pre>
riskProfileObjB<-calcAvgRiskAndProfile(clusObjB)
```

```
# compare clustering
compareClustering(riskProfileObjA,riskProfileObjB)
```

 ${\tt computeAssociatedVariable}$

compute Associated Variable

Description

computeAssociatedVariable.

Usage

compute Associated Variable (subject Values, clus Obj, cluster Plot Order, latex File=NULL)

Arguments

subjectValues dont know
clusObj dont know
clusterPlotOrder

dont know

latexFile dont know

Value

Need to look into this, I don't know how it compares them.

Author(s)

David Hastie and Silvia Liverani

 ${\tt computeRatioOfVariance}$

 $compute {\it Ratio Of Variance}$

Description

computeRatioOfVariance.

Usage

computeRatioOfVariance(runInfoObj)

Arguments

runInfoObj Object of type runInfoObj

Value

Need to look into this, I don't know how it compares them.

Author(s)

David Hastie and Silvia Liverani

generateSampleDataFile

Generate sample data files for profile regression

Description

•

Usage

generateSampleDataFile(clusterSummary)

Arguments

clusterSummary A vector of strings of the covariate names as by the column names in the data argument.

Value

The output of this function is a list with the following elements

yModel The outcome model according to which the data has been generated.

xModel The covariate model according to which the data has been generated.

inputData The data.frame that contains the data.

covNames The names of the covariates.

 ${\tt fixedEffectNames}$

The names of the fixed effects.

Author(s)

David Hastie and Silvia Liverani

is.wholenumber

Examples

is.wholenumber

Function to check if a number is a whole number

Description

Function to check if a number is whole, accounting for a rounding error.

Usage

```
is.wholenumber(x, tol = .Machine$double.eps^0.5)
```

Arguments

x The number to be checked.

tol Tolerance level.

Value

The default method for 'is.wholenumber' returns 'TRUE' if the number provided is a whole number.

Author(s)

David Hastie and Silvia Liverani

```
is.wholenumber(4) # TRUE
is.wholenumber(3.4) # FALSE
```

margModelPosterior 13

margModelPosterior

Marginal Model Posterior

Description

Compute the marginal model posterior.

Usage

```
margModelPosterior(runInfoObj)
```

Arguments

```
runInfoObj boh.
```

Value

It returns a number of files in the output directory as well as a list with the following elements.

Author(s)

Silvia Liverani

Examples

plotRiskProfile

Plot the Risk Profiles

Description

Plots the risk profiles for a profile regression model.

Usage

```
plotRiskProfile(riskProf0bj, outFile, showRelativeRisk=F,
    orderBy=NULL, whichClusters=NULL,
    whichCovariates=NULL, useProfileStar=F)
```

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Arguments

riskProfObj An object of type riskProfObj

outFile Path and file name to save the plot.

showRelativeRisk
Whether to show the relative risk.

orderBy Order by?

whichClusters Which clusters to show?
whichCovariates
Optional. Either a vector of indeces or a vector of strings that corresponds to the covariates that are to be displayed. The length of this vector must be greater

useProfileStar Whether to use Profile Star??

Value

Need to write this meanSortIndex

Author(s)

David Hastie and Silvia Liverani

```
# generation of data for clustering
## generation of fixed effects
fe1<-rnorm(200,0,1)
fe2<-runif(200,0,1)
## generation of the outcome
beta < -c(2,3)
W <- cbind(fe1,fe2)</pre>
theta<- c(-7,0,3)
clusterIndex<-c(rep(1,80),rep(2,60),rep(3,60))</pre>
mu<-theta[clusterIndex]+W</pre>
p<-1/(1+exp(-mu))
outcome<-vector()
for (i in 1:200){
    if(runif(1)<p[i]){</pre>
        outcome[i]<-1
    }else{
        outcome[i]<-0
## generation of the covariates
covariateProbs<-list(list(c(0.8,0.1,0.1),</pre>
    c(0.8, 0.1, 0.1),
    c(0.8, 0.1, 0.1),
    c(0.8, 0.1, 0.1),
    c(0.8,0.1,0.1)),
```

```
list(c(0.1,0.8,0.1),
    c(0.1,0.8,0.1),
    c(0.1,0.8,0.1),
    c(0.1,0.8,0.1),
    c(0.8,0.1,0.1)),
    list(c(0.8,0.1,0.1),
    c(0.1,0.1,0.8),
    c(0.1,0.1,0.8),
    c(0.1, 0.1, 0.8),
    c(0.1,0.1,0.8)))
X<-data.frame(Var1=rep(NA,200), Var2=rep(NA,200),</pre>
    Var3=rep(NA, 200), Var4=rep(NA, 200), Var5=rep(NA, 200))
for (i in 1:200){
    for (j in 1:5){
        u<-runif(1)</pre>
        for(kk in 1:3){
             if(u<cumsum(covariateProbs[[clusterIndex[i]]][[j]])[kk]){</pre>
                 X[i,j] < -kk-1
                 break
             }
        }
    }
}
inputData<-data.frame(cbind(outcome, X, fe1, fe2))</pre>
runInfoObj<-profRegr(yModel="Bernoulli", xModel="Discrete",
    nSweeps=100, nBurn=100, data=inputData, output="output",
    covNames=c("Var1","Var2","Var3","Var4","Var5"),
    fixedEffectsNames=c("fe1","fe2"))
dissimObj<-calcDissimilarityMatrix(runInfoObj)</pre>
clusObj<-calcOptimalClustering(dissimObj)</pre>
riskProfileObj<-calcAvgRiskAndProfile(clusObj)</pre>
clusterOrderObj<-plotRiskProfile(riskProfileObj, "summary.png",</pre>
    whichCovariates=c(1,2))
```

profRegr

Profile Regression

Description

Fit a profile regression model.

Usage

sampler="SliceDependent", alpha=-1, excludeY,
extraYVar, varSelectType, entropy,reportBurnIn=FALSE,
run=TRUE, discreteCovs, continuousCovs)

Arguments

covNames A vector of strings of the covariate names as by the column names in the data

argument.

fixedEffectsNames

A vector of strings of the fixed effect names as by the column names in the data

argument

outcome A string of column of the data argument that contains the outcome. The outcome

cannot have missing values - you could consider predicting the value of the

outcome for those subjects for which it has not been observed.

outcomeT A string of column of the data argument that contains the offset (for Poisson

outcome) or the number of trials (for Binomial outcome).

data A data frame which has as columns the outcome, the covariates, the fixed effects

if any and the offset (for Poisson outcome) or the number of trials (for Binomial outcome). The outcome cannot have missing values - you could consider predicting the value of the outcome for those subjects for which it has not been

observed.

output Path to folder to save all output files. The covariates can have missing values,

which must be coded as 'NA'. There cannot be missing values in the fixed effects

- if there are, use an imputation method before using profile regression.

hyper Path to file with hyperparameters specifications. This is optional: default values

are provided for all hyperparameters.

predict Data frame containing the predictive scenarios. See ?calcPredictions for more

details. This is only required if predictions are requested.

nSweeps Number of iterations of the MCMC after the burn-in period. By default this is

1000.

nBurn Number of initial iterations of the MCMC to be discarded. By default this is

1000.

reportBurnIn If TRUE then the burn in iterations are reported in the output files, if set to

FALSE they are not. It is set to FALSE by default.

nProgress The number of sweeps at which to print a progress update. By default this is

500.

nFilter The frequency (in sweeps) with which to write the output to file. The default

value is 1.

nClusInit The number of clusters individuals should be initially randomly assigned to

(Unif[50,60]).

seed The value for the seed for the random number generator. The default value is

the current time.

yModel The model type for the outcome variable. The options currently available are

"Bernoulli", "Poisson", "Binomial", "Categorical" and "Normal". The default

value is Bernoulli.

xModel The model type for the covariates. The options currently available are "Dis-

crete", "Normal" and "Mixed". The default value is "Discrete".

sampler The sampler type to be used. Options are "SliceDependent", "SliceIndependent"

and "Truncated". The default value is "SliceDependent".

alpha The value to be used if alpha is to remain fixed. If a negative value is used then

alpha is updated. The default value is -1.

excludeY If included only the covariate data X is modelled. By default this is not included. extraYVar If included extra Gaussian variance is included in the response model. By de-

fault the extra Gaussian variance is not included.

varSelectType The type of variable selection to be used "None", "BinaryCluster" or "Continu-

ous". The default value is "None".

entropy If included then we compute allocation entropy. By default the allocation en-

tropy is not included.

run Logical. If TRUE then the MCMC is run. Set run=FALSE if the MCMC has

been run already and it is only required to collect information about the run.

discreteCovs The names of the discrete covariates among the covariate names, if xModel="Mixed".

This and continuousCovs must be defined if xModel="Mixed", while covNames

is ignored.

continuousCovs The names of the discrete covariates among the covariate names, if xModel="Mixed".

This and continuousCovs must be defined if xModel="Mixed", while covNames

is ignored.

Value

It returns a number of files in the output directory as well as a list with the following elements.

directoryPath String. Directory path of the output files.

fileStem String. The

inputFileName String. Location and file name of input dataset as created by this function for

the C++ routines

nSweeps Integer. The number of sweeps of the MCMC after the burn-in.

nBurn Integer. The number of iterations in the burn-in period of the MCMC. reportBurnIn Logical. Whether the output of the burn-in report should be included.

nFilter Integer. The frequency (in sweeps) with which to write the output to file. The

default value is 1.

nSubjects Integer. The number of subjects.

nPredictSubjects

Integer. The number of subjects for which to run predictions.

covNames A vector of strings with the names of the covariates.

xModel String. The model type for the covariates.

includeResponse

Logical. If FALSE only the covariate data X is modelled.

yModel String. The model type for the outcome.

varSelect Logical. If FALSE no variable selection is performed.

varSelectType String. It specifies what type of variable selection has been performed, if any.

nCovariates Integer. The number of covariates.

nFixedEffects Integer. The number of fixed effects.

nCategoriesY Integer. The number of categories of the outcome, if yModel = "Categorical". It

is 1 otherwise.

nCategories Vector of integers. The number of categories of each covariate, if xModel =

"Discrete". It is 1 otherwise.

xMat A matrix of the covariate data.

yMat A matrix of the outcome data, including the offset if the outcome is Poisson and

the number of trials if the outcome is Binomial.

wMat A matrix of the fixed effect data.

Author(s)

David Hastie and Silvia Liverani

```
# example for Poisson outcome and Discrete covariates
inputs <- generateSampleDataFile(clusSummaryPoissonDiscrete())</pre>
runInfoObj<-profRegr(yModel=inputs$yModel,</pre>
    xModel=inputs$xModel, nSweeps=1000,
    nBurn=1000, data=inputs$inputData, output="output",
    covNames = inputs$covNames, outcomeT = inputs$outcomeT,
    fixedEffectsNames = inputs$fixedEffectNames)
dissimObj<-calcDissimilarityMatrix(runInfoObj)</pre>
clusObj<-calcOptimalClustering(dissimObj)</pre>
riskProfileObj<-calcAvgRiskAndProfile(clusObj)</pre>
clusterOrderObj<-plotRiskProfile(riskProfileObj, "summary.png")</pre>
# example with Bernoulli outcome and Mixed covariates
inputs <- generateSampleDataFile(clusSummaryBernoulliMixed())</pre>
runInfoObj<-profRegr(yModel=inputs$yModel,</pre>
    xModel=inputs$xModel, nSweeps=1000,
    nBurn=1000, data=inputs$inputData, output="output",
    discreteCovs = inputs$discreteCovs,
    continuousCovs = inputs$continuousCovs, nClusInit=10)
dissimObj<-calcDissimilarityMatrix(runInfoObj)</pre>
clusObj<-calcOptimalClustering(dissimObj)</pre>
riskProfileObj<-calcAvgRiskAndProfile(clusObj)</pre>
clusterOrderObj<-plotRiskProfile(riskProfileObj, "summary.png",</pre>
    whichCovariates=c(1,2,4,5))
```

summarise Var Select Rho 19

summariseVarSelectRho

Description

This function summarises the posterior distribution of rho, a parameter for variable selection only.

Usage

```
summariseVarSelectRho(runInfoObj)
```

Arguments

runInfo0bj Object of type runInfoObj

Value

A list with the following elements.

rho A matrix that has as many columns as the number of covariates and as many

rows as the number of sweeps. This matrix records the samples from the poste-

rior distribution of rho for each covariate at each sweep.

rhoMean Vector with the column means of the matrix rho above. Each value corresponds

to the posterior mean of rho for each covariate.

rhoMedian Vector with the column medians of the matrix rho above. Each value corre-

sponds to the posterior median of rho for each covariate.

rhoLowerCI Vector with the column lower confidence intervals of the matrix rho above. Each

value corresponds to the lower confidence interval of the posterior distribution

of rho for each covariate.

rhoUpperCI Vector with the column upper confidence intervals of the matrix rho above. Each

value corresponds to the upper confidence interval of the posterior distribution

of rho for each covariate.

Author(s)

David Hastie and Silvia Liverani

```
inputs <- generateSampleDataFile(clusSummaryVarSelectBernoulliDiscrete())
runInfoObj<-profRegr(yModel=inputs$yModel,
    xModel=inputs$xModel, nSweeps=100,
    nBurn=1000, data=inputs$inputData, output="output",
    covNames = inputs$covNames, varSelect="Continuous")
rho<-summariseVarSelectRho(runInfoObj)</pre>
```

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