# Package 'PReMiuM'

October 25, 2017

Type Package

Title Dirichlet Process Bayesian Clustering, Profile Regression

Version 3.1.5

Date 2017-10-24

**NeedsCompilation** yes

**Author** David I. Hastie, Silvia Liverani liveranis@gmail.com> and Sylvia Richardson with contributions from Aurore J. Lavigne, Lucy Leigh, Lamiae Azizi, Xi Liu, Ruizhu Huang

Maintainer Silvia Liverani liveranis@gmail.com>

Description Bayesian clustering using a Dirichlet process mixture model. This model is an alternative to regression models, non-parametrically linking a response vector to covariate data through cluster membership. The package allows Bernoulli, Binomial, Poisson, Normal, survival and categorical response, as well as Normal and discrete covariates. It also allows for fixed effects in the response model, where a spatial CAR (conditional autoregressive) term can be also included. Additionally, predictions may be made for the response, and missing values for the covariates are handled. Several samplers and label switching moves are implemented along with diagnostic tools to assess convergence. A number of R functions for post-processing of the output are also provided. In addition to fitting mixtures, it may additionally be of interest to determine which covariates actively drive the mixture components. This is implemented in the package as variable selection.

2 PReMiuM-package

# **R** topics documented:

PReM	iuM-package Dirichlet Process Bayesian Clustering	
Index		38
	vec2mat	3
	summariseVarSelectRho	
	setHyperparams	
	profRegr	
	plotRiskProfile	
	plotPredictions	
	margModelPosterior	
	mapforGeneratedData	
	is.wholenumber	
	heatDissMat	
	globalParsTrace	
	generateSampleDataFile	
	computeRatioOfVariance	
	clusSummaryBernoulliDiscrete	
	calcPredictions	
	calcOptimalClustering	8
	calcDissimilarityMatrix	- 1
	calcAvgRiskAndProfile	4
	PReMiuM-package	- 2

# **Description**

Dirichlet process Bayesian clustering and functions for the post-processing of its output.

# **Details**

Package: PReMiuM
Type: Package
Version: 3.1.5
Date: 2016-12-29
License: GPL2
LazyLoad: yes

Program to implement Dirichlet Process Bayesian Clustering as described in Liverani et al. 2014. This is a package for Bayesian clustering using a Dirichlet process mixture model. This model is an alternative to regression models, non-parametrically linking a response vector to covariate data through cluster membership. The package allows Bernoulli, Binomial, Poisson, Normal, survival and categorical response, as well as Normal and discrete covariates. It also allows for fixed effects in the response model, where a spatial CAR (conditional autoregressive) term can be also included.

PReMiuM-package 3

Additionally, predictions may be made for the response, and missing values for the covariates are handled. Several samplers and label switching moves are implemented along with diagnostic tools to assess convergence. A number of R functions for post-processing of the output are also provided. In addition to fitting mixtures, it may additionally be of interest to determine which covariates actively drive the mixture components. This is implemented in the package as variable selection.

The R package PReMiuM is supported through research grants. One key requirement of such funding applications is the ability to demonstrate the impact of the work we seek funding for can. Whatever you are using PReMiuM for, it would be very helpful for us to learn about our users, to tailor our future methodological developments to your needs. Please email us at liveranis@gmail.com or visit http://www.silvialiverani.com/support-premium/.

#### **Details**

# **PReMiuM** provides the following:

- Implements an infinite Dirichlet process model
- Can do dependent or independent slice sampling (Kalli et al., 2011) or truncated Dirichlet process model (Ishwaran and James, 2001)
- · Handles categorical or Normal covariates, or a mixture of them
- · Handles Bernoulli, Binomial, Categorical, Poisson, survival or Normal responses
- Handles inclusion of fixed effects in the response model, including a spatial CAR (conditional autoregressive) term
- Handles Extra Variation in the response (for Bernoulli, Binomial and Poisson response only)
- Handles variable selection (tested in Discrete covariate case only)
- Includes label switching moves for better mixing
- Allows user to exclude the response from the model
- Allows user to compute the entropy of the allocation
- Allows user to run with a fixed alpha or update alpha (default)
- Allows users to run predictive scenarios (at C++ run time)
- Basic or Rao-Blackwellised predictions can be produced
- · Handling of missing data
- C++ for model fitting
- Uses Eigen Linear Algebra Library and Boost C++
- Completely self contained (all library code in included in distribution)
- Adaptive MCMC where appropriate
- R package for generating simulation data and post processing
- R plotting functions allow user choice of what to order clusters by

#### **Authors**

David Hastie, Department of Epidemiology and Biostatistics, Imperial College London, UK Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Aurore J. Lavigne, Department of Epidemiology and Biostatistics, Imperial College London, UK Maintainer: Silvia Liverani < liveranis@gmail.com>

4 PReMiuM-package

#### Acknowledgements

Silvia Liverani thanks The Leverhulme Trust for financial support.

The R package PReMiuM is supported through research grants. One key requirement of such funding applications is the ability to demonstrate the impact of the work we seek funding for can. Whatever you are using PReMiuM for, it would be very helpful for us to learn about our users, to tailor our future methodological developments to your needs. Please email us at liveranis@gmail.com or visit http://www.silvialiverani.com/support-premium/.

# References

Molitor J, Papathomas M, Jerrett M and Richardson S. (2010) Bayesian Profile Regression with an Application to the National Survey of Children's Health, Biostatistics 11: 484-498.

Papathomas M, Molitor J, Richardson S. et al (2011) Examining the joint effect of multiple risk factors using exposure risk profiles: lung cancer in non smokers. Environmental Health Perspectives 119: 84-91.

Hastie, D. I., Liverani, S., Azizi, L., Richardson, S. and Stucker I. (2013) A semi-parametric approach to estimate risk functions associated with multi-dimensional exposure profiles: application to smoking and lung cancer. *BMC Medical Research Methodology*. 13 (1), 129.

Molitor, J., Brown, I. J., Papathomas, M., Molitor, N., Liverani, S., Chan, Q., Richardson, S., Van Horn, L., Daviglus, M. L., Stamler, J. and Elliott, P. (2014) Blood pressure differences associated with DASH-like lower sodium compared with typical American higher sodium nutrient profile: IN-TERMAP USA. Hypertension 64 (6), 1198-1204. Available at http://www.ncbi.nlm.nih.gov/pubmed/25201893

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

Hastie, D. I., Liverani, S. and Richardson, S. (2014) Sampling from Dirichlet process mixture models with unknown concentration parameter: Mixing issues in large data implementations. *Statistics* & *Computing*. Available at http://link.springer.com/article/10.1007

calcAvgRiskAndProfile Calculation of the average risks and profiles

# **Description**

Calculation of the average risks and profiles.

# Usage

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

#### **Arguments**

clus0bj Object of type clusObj.

includeFixedEffects

By default this is set to FALSE. If it is set to FALSE then the risk profile is computed with the parameters beta of the fixed effects assumed equal to zero. If it is set to TRUE, then risk profile at each sweep is computed adjusting for the sample of the beta parameter at that sweep.

proportionalHazards

Whether the risk matrix should include lambda only for the yModel="Survival" case so that the proportional hazards can be computed in the plotting function. The default is the average survival time.

#### Value

A list with the following components. This is an object of type riskProfileObj.

riskProfClusObj

profile

The object of type clusObj as given in the input of this function.

risk A matrix that has a column for each cluster and a row for each sweep. Each element of the matrix represents the estimated risk at each sweep for each cluster.

An array whose first dimension is the number of sweeps, the second is the number of clusters, the third is the number of discrete covariates and the fourth is the

ber of clusters, the third is the number of discrete covariates and the fourth is the number of categories of each of the covariates. Each element of the array represents the covariate profile at each sweep for each cluster. The fourth dimension does not exists if the covariate type is Normal. If the covariate type is mixed, then instead of this element, the two elements below are defined, 'profilePhi'

and 'profileMu'.

profileStar This is NULL if there has not been any variable selection. otherwise it contains

the

empiricals A vector of length of the optimal number of clusters, where each value is the

empirical mean of the outcome for each cluster.

profileStdDev An array whose first dimension is the number of sweeps, the second is the num-

ber of clusters, the third and the fourth are the number of continuous covariates. Each square matrix identified by the first and second dimension of the array represents the standard deviation at each sweep for each cluster. This element is

only available if the covariate type is continuous or mixed.

profilePhi This array is the equivalent of the 'profile' above for discrete covariates in case

of mixed covariates.

profileStarPhi This array is defined as profile and profilePhi, but the values are computed only

if a variable selection procedure has been run. The definition of the star profile is given in Liverani, S., Hastie, D. I. and Richardson, S. (2013) PReMiuM: An

R package for Bayesian profile regression.

profileMu This array is the equivalent of the 'profile' above for Normal covariates in case

of mixed covariates.

profileStarMu This array is defined as profile and profileMu, but the values are computed only

if a variable selection procedure has been run. The definition of the star profile is given in Liverani, S., Hastie, D. I. and Richardson, S. (2013) PReMiuM: An

R package for Bayesian profile regression.

nuArray For yModel=Survival when weibullFixedShape=FALSE this array contains the

sampled values of the shape parameter nu. The first dimension is the number of

sweeps, the second is the number of clusters.

#### Authors

David Hastie, Department of Epidemiology and Biostatistics, Imperial College London, UK Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC

Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani eranis@gmail.com>

# References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

calcDissimilarityMatrix

Calculates the dissimilarity matrix

#### **Description**

Calculates the dissimilarity matrix.

# Usage

calcDissimilarityMatrix(runInfoObj, onlyLS=FALSE)

# **Arguments**

runInfo0bj Object of type runInfoObj.

onlyLS Logical. It is set to FALSE by default. When it is equal to TRUE the dissimilar-

ity matrix is not returned and the only method available to identify the optimal partition using 'calcOptimalClustering' is least squares. This parameter is to be used for datasets with many subjects, as C++ can compute the dissimilarity matrix but it cannot pass it to R for usage in the function 'calcOptimalClustering'. As guidance, be aware that a dataset with 85,000 subjects will require a RAM

of about 26Gb, even if onlyLS=TRUE.

# 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).

onlyLS Logical. If it set to TRUE the only method available to identify the optimal

partition using 'calcOptimalClustering' is least squares.

#### **Authors**

David Hastie, Department of Epidemiology and Biostatistics, Imperial College London, UK

Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC

Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani diveranis@gmail.com>

#### References

Liverani, S., Hastie, D. I., Azizi, L., Papathomas, M. and Richardson, S. (2014) PReMiuM: An R package for Profile Regression Mixture Models using Dirichlet Processes. *Forthcoming in the Journal of Statistical Software*. Available at http://uk.arxiv.org/abs/1303.2836

#### **Examples**

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). Note that this is set to TRUE by default if disSimObj\$onlyLS

is set to TRUE.

#### Value

the output is a list with the following elements. This is an object of type clusObj.

clusObjRunInfoObj

Details on this run. An object of type runInfoObj.

clusterSizes Cluster sizes.

clusteringPred The predicted cluster memberships for the predicted scenarios.

clusObjDisSimMat

Dissimilarity matrix.

clustering Cluster memberships.

nClusters Optimal number of clusters.

avgSilhouetteWidth

Average silhouette width when using medoids method for clustering.

#### **Authors**

David Hastie, Department of Epidemiology and Biostatistics, Imperial College London, UK

Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani liveranis@gmail.com>

#### References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

# **Examples**

calcPredictions

Calculates the predictions

# **Description**

Calculates the predictions.

# Usage

```
calcPredictions(riskProfObj, predictResponseFileName=NULL,
    doRaoBlackwell=F, fullSweepPredictions=F, fullSweepLogOR=F,
    fullSweepHazardRatio=F,referenceClusterOR=NA)
```

#### **Arguments**

riskProf0bj Object of type riskProf0bj.

predictResponseFileName

If this function is run after the function profRegr, and outcome (and possibly fixed effects) are known for the predicted profiles, then there is no need to set this, as the function profRegr will have produced a file ending in "\_predict-Full.txt". This file allows the computation of measures of fit for cross-validation. If the file has not been produced automatically, it can be produced manually and it can be provided here. We discourage this and we provide no documentation for doing so.

doRaoBlackwell By default this is set to FALSE. If it is set to TRUE then Rao-Blackwell predictions are computed.

fullSweepPredictions

By default this is set to FALSE. If it is set to TRUE then a prediction is computed for each sweep.

fullSweepLogOR By default this is set to FALSE. If it is set to TRUE then a prediction log OR is computed for each sweep.

fullSweepHazardRatio

By default this is set to FALSE. If it is set to TRUE then a prediction hazard ratio is computed for each sweep, only for Survival response.

referenceClusterOR

The cluster of reference for the odds ratios. If this is not provided then the first of the predictive profiles provided is used as the reference.

# Value

The output is a list with the following elements.

bias The bias of the predicted values with respect to the observed outcome. If the

response is not provided, this is set to NA.

rmse The root mean square error of the predicted values with respect to the observed

outcome. If the response is not provided, this is set to NA.

mae The mean absolute error of the predicted values with respect to the observed

outcome. If the response is not provided, this is set to NA.

observedY The values of the outcome provided by the user. This is in the case that predic-

tions are run as a validation tool. If the response is not provided, this is set to

NA.

predictedY This matrix has as many rows as predictions requested by the user. It is the

median of the predicted values over all the sweeps that have been run after the

burn-in period.

doRaoBlackwell This is set to TRUE if it has done Rao-Blackwell predictions, and FALSE oth-

erwise.

predictedYPerSweep

This array has the first dimension equivalent to the number of sweeps and the second dimension as large as the number of predictions requested by the user. It contains the predicted values per sweep.

logORPerSweep This array has the first dimension equivalent to the number of sweeps and the

second dimension as large as the number of predictions requested by the user. It contains the predicted log OR values per sweep (not available for Poisson and

Normal outcome).

fullHR This array has the first dimension equivalent to the number of sweeps and the

second dimension as large as the number of predictions requested by the user. It contains the predicted hazard ratio values per sweep (only for Survival out-

come).

#### **Details**

This functions computes predicted responses, for various prediction scenarios. It is assumed that the predictive allocations and Rao-Blackwell predictions have already been done in profRegr using the 'predict' input.

The user can provide the function profRegr with a data.frame through the predict argument. This data.frame has 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 data.frame are denoted by 'NA'. If the data.frame 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. If the response is provided in the data frame it must be in a column called "outcome".

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.

# Authors

David Hastie, Department of Epidemiology and Biostatistics, Imperial College London, UK

Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani liveranis@gmail.com>

#### References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

```
## Not run:
inputs <- generateSampleDataFile(clusSummaryBernoulliDiscrete())
# prediction profiles
preds<-data.frame(matrix(c(0, 0, 1, 0, 0,</pre>
```

```
0, 0, 1, NA, 0), ncol=5, byrow=TRUE))
colnames(preds)<-names(inputs$inputData)[2:(inputs$nCovariates+1)]</pre>
# run profile regression
runInfoObj<-profRegr(yModel=inputs$yModel, xModel=inputs$xModel,</pre>
    nSweeps=100, nBurn=1000, data=inputs$inputData, output="output",
    covNames=inputs$covNames,predict=preds)
# postprocessing
dissimObj <- calcDissimilarityMatrix(runInfoObj)</pre>
clusObj <- calcOptimalClustering(dissimObj)</pre>
riskProfileObj <- calcAvgRiskAndProfile(clusObj)</pre>
clusterOrderObj <- plotRiskProfile(riskProfileObj, "summary.png",</pre>
    whichCovariates=c(1,2))
output_predictions <- calcPredictions(riskProfileObj,fullSweepPredictions=TRUE)</pre>
# example where the fixed effects can be provided for prediction
# but the observed response is missing
# (there are 2 fixed effects in this example).
# in this example we also use the Rao Blackwellised predictions
inputs <- generateSampleDataFile(clusSummaryPoissonNormal())</pre>
# prediction profiles
predsPoisson<- data.frame(matrix(c(7, 2.27, -0.66, 1.07, 9,
     -0.01, -0.18, 0.91, 12, -0.09, -1.76, 1.04, 16, 1.55, 1.20, 0.89,
     10, -1.35, 0.79, 0.95), ncol=5, byrow=TRUE))
colnames(predsPoisson)<-names(inputs$inputData)[2:(inputs$nCovariates+1)]</pre>
# run profile regression
runInfoObj<-profRegr(yModel=inputs$yModel,</pre>
         xModel=inputs$xModel, nSweeps=100,
         nBurn=100, data=inputs$inputData, output="output",
         covNames = inputs$covNames, outcomeT="outcomeT",
         fixedEffectsNames = inputs$fixedEffectNames,predict=predsPoisson)
# postprocessing
dissimObj<-calcDissimilarityMatrix(runInfoObj)</pre>
clusObj<-calcOptimalClustering(dissimObj)</pre>
riskProfileObj<-calcAvgRiskAndProfile(clusObj)</pre>
output_predictions <- calcPredictions(riskProfileObj,fullSweepPredictions=TRUE)</pre>
# example where both the observed response and fixed effects are present
#(there are no fixed effects in this example, but
# these would just be added as columns between the first and last columns).
inputs <- generateSampleDataFile(clusSummaryPoissonNormal())</pre>
# prediction profiles
predsPoisson<- data.frame(matrix(c(NA, 2.27, -0.66, 1.07, NA,
     -0.01, -0.18, 0.91, NA, -0.09, -1.76, 1.04, NA, 1.55, 1.20, 0.89,
     NA, -1.35, 0.79, 0.95), ncol=5, byrow=TRUE))
```

```
colnames(predsPoisson)<-names(inputs$inputData)[2:(inputs$nCovariates+1)]</pre>
 # run profile regression
 runInfoObj<-profRegr(yModel=inputs$yModel,</pre>
           xModel=inputs$xModel, nSweeps=10,
           nBurn=20, data=inputs$inputData, output="output",
           covNames = inputs$covNames, outcomeT="outcomeT",
           fixedEffectsNames = inputs$fixedEffectNames,
           nClusInit=15, predict=predsPoisson)
 # postprocessing
 dissimObj<-calcDissimilarityMatrix(runInfoObj)</pre>
 clusObj<-calcOptimalClustering(dissimObj)</pre>
 riskProfileObj<-calcAvgRiskAndProfile(clusObj)</pre>
 output_predictions <- calcPredictions(riskProfileObj,fullSweepPredictions=TRUE)</pre>
 ## End(Not run)
clusSummaryBernoulliDiscrete
                          Sample datasets for profile regression
```

#### **Description**

Definition of skeleton of sample datasets for profile regression.

# Usage

```
clusSummaryBernoulliDiscrete()
clusSummaryBernoulliNormal
clusSummaryBernoulliDiscreteSmall()
clusSummaryBinomialNormal()
clusSummaryCategoricalDiscrete()
clusSummaryNormalDiscrete()
clusSummaryNormalNormal()
clusSummaryNormalNormalSpatial()
clusSummaryPoissonDiscrete()
clusSummaryPoissonNormal()
clusSummaryPoissonNormalSpatial()
clusSummaryPoissonNormalSpatial()
clusSummaryVarSelectBernoulliDiscrete()
clusSummaryWeibullDiscrete()
clusSummaryWeibullDiscrete()
clusSummaryQuantileNormal()
```

# Value

The output of these function is a list with the following components. These can be used as inputs for profile regression function profRegr().

outcomeType The outcome type of the dataset.

CovariateType The covariate type of the dataset.

 ${\tt nCovariates} \qquad \text{The number of covariates generated}.$ 

nCategories The number of categories of the covariates if the covariates are discrete or mixed.

nFixedEffects The number of fixed effects.

fixedEffectsCoeffs

The names of the fixed effects.

missingDataProb

The pobability of generating missing data.

nClusters The number of clusters.

clusterSizes The number of observations in each cluster.

clusterData The dataset, including the outcome, the covariates, the fixed effects, the number

of trials (if Binomial outcome) and the offset (for Poisson outcome).

covNames The names of the covariates of the dataset.

nDiscreteCovs The number of discrete covariates, if the covariate type is mixed.

nContinuousCovs

The number of continuous covariates, if the covariate type is mixed.

outcomeT The name of the column of the dataset containing the number of trials (if Bino-

mial outcome) or the offset (for Poisson outcome).

includeCAR A boolean specifying wether a spatial CAR term is included.

TauCAR The precision for the spatial CAR term.

# Details

clusSummaryBernoulliDiscrete generates a dataset with Bernoulli outcome and discrete covariates.

clusSummaryBernoulliNormal generates a dataset with Bernoulli outcome and Normal covariates.

clusSummaryBernoulliDiscreteSmall generates a dataset with Bernoulli outcome and discrete covariates (with smaller cluster sizes).

clusSummaryBinomialNormal generates a dataset with Binomial outcome and discrete covariates.

clusSummaryCategoricalDiscrete generates a dataset with categorical outcome and discrete covariates.

clusSummaryNormalDiscrete generates a dataset with Normal outcome and discrete covariates.

clusSummaryNormalNormal generates a dataset with Normal outcome and Normal covariates.

clusSummaryNormalNormalSpatial generates a dataset with Normal outcome, Normal covariates and a spatial conditional autoregressive term in the log relative risk.

clusSummaryPoissonDiscrete generates a dataset with Poisson outcome and discrete covariates.

clusSummaryPoissonNormal generates a dataset with Poisson outcome and Normal covariates.

clusSummaryPoissonNormalSpatial generates a dataset with Poisson outcome, Normal covariates and a spatial conditional autoregressive term in the log relative risk.

clusSummaryVarSelectBernoulliDiscrete generates a dataset with Bernoulli outcome and discrete covariates, suitable for variable selection as some covariates are not driving the clustering.

clusSummaryBernoulliMixed generates a dataset with Bernoulli outcome and mixed covariates. clusSummaryWeibullDiscrete generates a dataset with a Weibull outcome and censored observa-

tions.

clusSummaryQuantileNormal generates a dataset with a Quantile outcome and censored observations.

#### **Authors**

David Hastie, Department of Epidemiology and Biostatistics, Imperial College London, UK Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Aurore J. Lavigne, Department of Epidemiology and Biostatistics, Imperial College London, UK Maintainer: Silvia Liverani < liveranis@gmail.com>

#### References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

#### **Examples**

names(clusSummaryBernoulliDiscrete())

computeRatioOfVariance

computeRatioOfVariance

# Description

Computes of the ratio between the variance of the extra variation and the total variance.

# Usage

computeRatioOfVariance(runInfoObj)

#### **Arguments**

This function can only be used when the extra variation is included in the response model.

Object of type runInfoObj

# Value

runInfoObj

For each sweep this function outputs the ratio between the variance of the thetas' and the sum of the variances of the thetas' and the extra variation epsilon as described in Liverani et al. (2013).

#### **Authors**

David Hastie, Department of Epidemiology and Biostatistics, Imperial College London, UK Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani liveranis@gmail.com>

#### References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

generateSampleDataFile

Generate sample data files for profile regression

# **Description**

Generation of random sample datasets for profile regression.

#### Usage

```
generateSampleDataFile(clusterSummary, pQuantile=0.05)
```

#### **Arguments**

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

argument.

pQuantile pQuantile parameter of the Asymmetric Laplace Distribution used

to generate data to test the model for the quantiles.

#### 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.

uCAR The spatial gaussian effect. It is sample into the intrinsic autoregressive model

with precision TauCAR under the constraint that the sum of term is null. Only

used if includeCAR is TRUE.

TauCAR The precision of the spatial CAR effect. Only used if includeCAR is TRUE.

globalParsTrace 17

Permutation

A vector of size nSubject given the cluster name of each subject. When spatial CAR is added to the model, for preventing potential identifiability problems, the clusters are randomly distributed within the all subjects. Only used if include-CAR is TRUE.

#### **Authors**

David Hastie, Department of Epidemiology and Biostatistics, Imperial College London, UK Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Aurore J. Lavigne, Department of Epidemiology and Biostatistics, Imperial College London, UK Maintainer: Silvia Liverani < liveranis@gmail.com>

#### References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

#### **Examples**

```
# generation of data for clustering
generateDataList <- clusSummaryBernoulliDiscrete()
inputs <- generateSampleDataFile(generateDataList)</pre>
```

globalParsTrace

Plot of the trace of some of the global parameters

#### **Description**

Function to lot the trace of some global parameters

#### Usage

globalParsTrace(runInfoObj, parameters = "nClusters",plotBurnIn=FALSE,whichBeta=1)

#### **Arguments**

This function allows to visualise the trace of the global parameters. Note that this function has not been optimised for large datasets.

An object of class runInfoObj.

panām€o⊖bs

The parameter whose trace will be plotted. This can be set equal to "nClusters" (default), "alpha", "mpp" and "beta", as by the model. As beta can be a vector, we advise to also set the option "whichBeta" below to select which fixed effect parameter to visualise in the plot. "mpp" stands for marginal partition posterior, also referred to as marginal model posterior.

18 heatDissMat

plotBurnIn Set to FALSE (default) it does not plot the trace for the burn in period. Set to

TRUE it plots the trace including the burn in period.

whichBeta Integer which selects which fixed effect parameter is plotted.

#### Value

Plot of trace of some global parameters.

#### **Authors**

Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani liveranis@gmail.com>

#### References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

#### **Examples**

heatDissMat

Plot the heatmap of the dissimilarity matrix

# Description

Function to plot the heatmap of the dissimilarity matrix

# Usage

```
heatDissMat(dissimObj, main=NULL, xlab=NULL, ylab=NULL)
```

heatDissMat 19

# **Arguments**

dissimObj	An object of class dissimObj.
main	The usual plot option, to be passed to the heatmap function.
ylab	The usual plot option, to be passed to the heatmap function.
xlab	The usual plot option, to be passed to the heatmap function.

#### Value

Plot of the heatmap of the dissimilary matrix. This functions uses the function 'heatmap' of package 'stats'. Note that this function has not been optimised for large datasets.

#### Authors

Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani liveranis@gmail.com>

#### References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

```
## Not run:
# generate simulated dataset
generateDataList <- clusSummaryBernoulliDiscreteSmall()
inputs <- generateSampleDataFile(generateDataList)

# run profile regression
runInfoObj<-profRegr(yModel=inputs$yModel, xModel=inputs$xModel,
nSweeps=10, nBurn=2000, data=inputs$inputData, output="output",
covNames=inputs$covNames,nClusInit=15)

# compute dissimilarity matrix
dissimObj<-calcDissimilarityMatrix(runInfoObj)

# plot heatmap
heatDissMat(dissimObj)

## End(Not run)</pre>
```

20 is, wholenumber

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**

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.

#### **Authors**

David Hastie, Department of Epidemiology and Biostatistics, Imperial College London, UK

Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani diveranis@gmail.com>

#### References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

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

mapforGeneratedData 21

mapforGeneratedData I	Мар	generated data
-----------------------	-----	----------------

# **Description**

Function to draw the map of a vector when data are generated.

# Usage

```
mapforGeneratedData(u, del=NULL, palette='RGB', main='' )
```

# **Arguments**

u	A vector of size nSubject to map. The function is only useful when data are generated by generateSampleDataFile.
del	A numeric vector of increasing order given the breaks to color the map. By default the centiles of u are used.
palette	Color palette to be used. Either 'RGB' (default) Red-Green-Blue, or 'BW' for black and white.
main	A string for title.

#### **Authors**

Aurore J. Lavigne, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani liveranis@gmail.com>

#### References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

# **Examples**

 $inputs = generate Sample Data File (clus Summary Poisson Normal Spatial ()) \\ map for Generated Data (inputs $uCAR)$ 

22 margModelPosterior

margModelPosterior

Marginal Model Posterior

#### **Description**

Compute the marginal model posterior.

#### Usage

```
margModelPosterior(runInfoObj,allocation)
```

#### **Arguments**

runInfo0bj An object of type runInfoObj.

allocation By default, if allocation is not provided, the \_z.txt file is read to compute the

marginal model posterior for all the partitions available there. If allocation is equal to a vector that corresponds to a partition, the marginal model posterior is

computed for that given partition.

#### Value

It returns a file in the output folder, with name ending in "\_margModPost.txt", that contains the marginal model posterior. It also returns a list. The first argument is called margModPost and it is the mean of the values of the marginal model posterior as they appear in the file ending in "\_margModPost.txt" in the output folder. The second argument is an updated runInfoObj which also include some hyperparameter values.

#### **Authors**

Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani liveranis@gmail.com>

#### References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

plotPredictions 23

margModelPosterior(runInfoObj)

# **Description**

Plots the conditional density for the predicted scenarios provided. It produces a pdf with a page for each predictive scenario provided. Each page has a plot of the predicted response, in the order as they were provided to the function. Note that fixed effects are not processed in this function. This function has been developed for Bernoulli, Normal and Survival response only. This function has been developed for Discrete and Normal covariates only.

# Usage

#### **Arguments**

outfile	String. The name of the output PDF file. The default is "condDensity.pdf".
runInfoObj	An object of type runInfoObj which contains all the details about the run of profRegr.
predictions	An object of type predictions which contains all the details about the run of calcPredictions.
logOR	Whether to plot the response probability or log odds ratios. The default is FALSE and the response probability is plotted.

# Value

The output is a plot in PDF format.

#### Authors

Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani eranis@gmail.com>

# References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

24 plotRiskProfile

#### **Examples**

```
## Not run:
# example with Bernoulli outcome and Discrete covariates
inputs <- generateSampleDataFile(clusSummaryBernoulliDiscrete())</pre>
# prediction profiles
preds<-data.frame(matrix(c(</pre>
2, 2, 2, 2, 2,
0, 0, NA, 0, 0), ncol=5, byrow=TRUE))
colnames(preds)<-names(inputs$inputData)[2:(inputs$nCovariates+1)]</pre>
# run profile regression
runInfoObj<-profRegr(yModel=inputs$yModel, xModel=inputs$xModel,</pre>
nSweeps=10000, nBurn=10000, data=inputs$inputData, output="output",
covNames=inputs$covNames,predict=preds,
fixedEffectsNames = inputs$fixedEffectNames)
dissimObj <- calcDissimilarityMatrix(runInfoObj)</pre>
clusObj <- calcOptimalClustering(dissimObj)</pre>
riskProfileObj <- calcAvgRiskAndProfile(clusObj)</pre>
predictions <- calcPredictions(riskProfileObj,fullSweepPredictions=TRUE,fullSweepLogOR=TRUE)</pre>
plotPredictions(outfile="predictiveDensity.pdf",runInfoObj=runInfoObj,
predictions=predictions,logOR=TRUE)
## End(Not run)
```

plotRiskProfile

Plot the Risk Profiles

#### **Description**

Plots the risk profiles for a profile regression model.

# Usage

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

# Arguments

riskProfObj An object of type riskProfObj.

outFile Path and file name to save the plot.
showRelativeRisk

Whether to show the relative risk (with respect to the risk of the first cluster). This option is not available for Normal outcome. For Survival outcomes it computed proportional hazards, but only if the option proportionalHazards=T was used in the function calcAvgRiskAndProfile().

plotRiskProfile 25

orderBy Order by which the clusters are to be displayed. It can take values "Empirical",

> "ClusterSize" and "Risk" (the latter only if the outcome is provided). It can also take the name of a covariate to order the clusters, in which case the clusters are

ordered.

whichClusters Either a vector of indeces that corresponds to the clusters that are to be displayed.

The length of this vector must be greater than 1. The default is that all clusters

are shown.

whichCovariates

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 than 1. The

default is that all covariates are shown.

useProfileStar To be set equal to TRUE only if a variable selection procedure has been run. The

definition of the star profile is given in Liverani, S., Hastie, D. I. and Richardson,

S. (2013) PReMiuM: An R package for Bayesian profile regression.

riskLim Limits of the y-axis for the plot of the boxplots for the response variable. The

default is NULL. If the riskLim are provided, they should be a vector of length

#### Value

This function creates a png plot saved in the path given by outFile. All clusters are visually displayed together.

For discrete covariates, instead of plotting the probability that a phi is above or below the mean value, we plot the actual phi values (and plot the mean value across clusters as a horizontal line).

For normal covariates, for each covariate the upper plot is the posterior distribution for the mean mu, and the lower plot is the posterior distribution of sqrt(Sigma[i,i]) (i.e. the standard deviation for that covariate).

It also returns the following vector.

This vector is the index that represents the order that the clusters are represented. meanSortIndex

The default ordering is by empirical risk.

#### **Authors**

David Hastie, Department of Epidemiology and Biostatistics, Imperial College London, UK

Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani liveranis@gmail.com>

#### References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

#### **Examples**

profRegr

Profile Regression

# Description

Fit a profile regression model.

# Usage

# Arguments

covNames

A vector of strings of the covariate names as by the column names in the data argument. The names of the covariates cannot include space characters.

fixedEffectsNames

A vector of strings of the fixed effect names as by the column names in the data argument. Each fixed effect must be of class 'numeric'. If a fixed effect is of class 'character', an error message will appear and the fixed effect will need to be recoded as numeric. The names of the fixed effects cannot include space characters.

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. The name cannot include space characters.

outcomeT

A string of column of the data argument that contains the offset (for Poisson outcome) or the number of trials (for Binomial outcome) or censoring for Survival reponse (coded as 0 or 1). The name cannot include space characters.

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) or censoring (for Survival 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. For Survival response censoring must be coded as 0 if the event has not occurred (ie, there has been censoring) and 1 if the event has occurred (no censoring has taken place). The names of the columns cannot include space characters.

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

Object of type setHyperparams with hyperparameters specifications. This is optional, default values are provided for all hyperparameters. See ?setHyperparams for details.

predict

Data frame containing the predictive scenarios. This is only required if predictions are requested.

At each iteration the predictive subjects are assigned to one of the current clusters according to their covariate profiles (but ignoring missing values), or their Rao Blackwellised estimate of theta is recorded (a weighted average of all theta, weighted by the probability of allocation into each cluster. For Normal and Quantile response they can also be randomly allocated. See also the option predictType below.

The predictive subjects have no impact on the likelihood and so do not determine the clustering or parameters at each iteration. The predictive allocations are then recorded as extra entries in each row of the output\_z.txt file. This can then be processed in the post processing to create a dissimilarity matrix with the fitting subjects. The post procesing function calcPredictions will create predicted response values for these subjects.

See ?calcPredictions for more details and examples.

predictType

This can be set equal to "RaoBlackwell" and "random". The default is RaoBlackwell. The random option can only be used for Normal and Quantile response, where the estimated variance of the clusters is considered and the predictive subjects are randomly assigned to a mixture component and then are also randomly sampled within that component.

nSweeps

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

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", "Normal", "Quantile" and

"Survival". 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 fixed. If a value smaller than or equal to -1 is used

then alpha is random, if dPitmanYor is equal to zero (the random alpha option is available for Dirichlet process prior only). The default value is -2 (random alpha). For fixed alpha, if dPitmanYor is in the interval (0,1) then a Pitman-Yor

process prior is used instead of a Dirichlet process prior.

dPitmanYor The discount parameter for the Pitman-Yor process prior. The default value is

0, which is equivalent to a Dirichlet process prior. This parameter must belong to the interval [0,1) and it must be provided together with a non-negative value for alpha. The Pitman-Yor process prior is only available for non-random parameters. Note that the third label switching move is only available for Dirichlet process priors, so it will not be run if dPitmanYor>0. Therefore setting dPit-

manYor to a value greater than zero will forse whichLabelSwitch=12.

excludeY If TRUE only the covariate data X is modelled. By default this is set to FALSE.

extraYVar If set equal to TRUE extra Gaussian variance is included in the response model. This option is available only for Bernoulli, Binomial and Poisson response. By

default the extra Gaussian variance is not included, so extraYVar=FALSE.

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

tinuous". The "Continuous" variable selection is the implementation of the novel variable selection formulation proposed by Papathomas, Molitor, Hoggart, Hastie, Richardson (2012) "Exploring data from genetic association studies using Bayesian variable selection and the Dirichlet process: application to searching for gene x gene patterns" in Genetic Epidemiology. The "BinaryCluster" variable selection is based on the method proposed by Chung and Dunson (2009) "Nonparametric Bayes conditional distribution modelling with variable selection" in the Journal of the American Statistical Association. Both types of variable selection can be used with discrete, continuous or mixed covariates.

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.

whichLabelSwitch

The label switching moves to run. The options available are moves 1, 2 and 3 ("123"), moves 1 and 2 ("12") and move 3 only ("3"). The moves are described in Hastie et al. (2013). Note that the third label switching move is only available for Dirichlet process priors, so it will not be run if dPitmanYor>0. Therefore setting dPitmanYor to a value greater than zero will forse whichLabelSwitch=12.

includeCAR A boolean specifying wether a conditional autoregressive term should be intro-

duced within the model, to take into account possible spatial correlation within

residuals. Only for Poisson and Normal response models.

neighboursFile The file name of the file specifying neighbourhood graph. It should have the

same structure than neighbourhood graph files used in the "INLA" package, and can be produced from a nb object of package "spdep", by the function "nb2INLA" of package "spdep". See ?nb2INLA for details. Each file must

have at least one neighbour.

uCARinit This parameter gives the possibility of giving initialisation values for the spatial

residuals u of the spatial CAR. It is set to FALSE by default (meaning that the spatial residuals are initialised randomly). It can be set alternatively to a vector

of values, one for each of the observations available.

weibullFixedShape

This parameter controls whether the shape parameter of the Weibull distribution (for yModel=Survival only) is a global parameter (fixed) or cluster specific. It is

equal to TRUE by default.

useNormInvWishPrior

By default this variable equals FALSE. When this variable equals TRUE, the conjugate Normal-inverse-Wishart prior is used rather than the independent normal and inverse Whishart priors. If this prior is used, variable selection cannot

be used as it has not been implemented.

#### Value

Once the C++ has completed the output from fitting the regression is stored in a number of text files in the directory specified. Files are produced containing the MCMC traces for all of the values of interest, along with a log file and files for monitoring the acceptance rates of the adaptive Metropolis Hastings moves.

It returns a number of files in the output directory as well as a list with the following elements. This an object of type runInfoObj. The files that are produced in the output directory are described below.

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.

nProgress The number of sweeps at which to print a progress update.

nSubjects Integer. The number of subjects.

nPredictSubjects

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

fullPredictFile

Logical. It is FALSE by default. It is equal to TRUE if the outcome or the outcome and the fixed effects were included in the dataframe provided in the input predict. If TRUE, the function will have a produced a file ending in "\_predictFull.txt" which contains the values of the outcome and fixed effects for the

computation of measures of fit in the function calcPredictions.

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.

extraYVar TRUE if extra Gaussian variance is included in the response model.

xMat A matrix of the covariate data.

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

number of trials if the outcome is Binomial and 0 or 1 for Survival outcome (1

for censored individuals, 0 otherwise).

wMat A matrix of the fixed effect data.

whichLabelSwitch

The label switching moves that have been run. The options available are moves 1, 2 and 3 ("123"), moves 1 and 2 ("12") and move 3 only ("3"). The moves are

described in Hastie et al. (2013).

includeCAR Logical. Whether a spatial CAR term is included.

predictType String. Whether a RaoBlackwell or random predictions have been computed. weibullFixedShape

Logical. Whether the shape parameter of the Weibull distribution for the survival response is fixed or cluster specific.

These are the files produced in the output directory. We refer to Liverani et al. (2015)

_alpha.txt	If alpha is random, each row is a draw from a posterior distribution of alpha (including burn in if reportBurnIn=TRUE).
_beta.txt	If fixed effects are included, this file provides the draws from the posterior distribution of the beta parameters at each sweep. Each row represents the vector of beta's at each sweep (including burn in if reportBurnIn=TRUE).
_hyper.txt	Internal file to communicate between R and C++ the values of the hyperparamters.
_input_txt	Internal file to communicate the data between R and C++.
_log.txt	This file logs some information about the run, such as what variables were included, which hyperparameters were used, the seed of the random numbers, the acceptance rates of the MCMC moves that were included in the run.
_logPost.txt	This file report the logPosterior, the logLikelihood and logPrior for the model fit at each sweep (including burn in if reportBurnIn=TRUE).
_nClusters.txt	This file includes the number of clusters at each sweep. Each row represents a sweep (including burn in if reportBurnIn=TRUE) and each element in the rows is the number of clusters per sweep. This includes the number of empty clusters, if any.
_nMembers.txt	This file includes the number of observations in each cluster at each sweep. Each row represents a sweep (including burn in if reportBurnIn=TRUE) and each element in the rows is the number of observations in each cluster per sweep. The last number in each row is the total number of observations, computed as the sum of the elements in the row as a check that all observations have been assigned to a cluster.
_theta.xt	This file includes the value of theta (cluster specific parameter for the response variable) for each cluster at each sweep. Each row represents a sweep (including burn in if reportBurnIn=TRUE) and each element in the rows is the value of theta for each cluster at that sweep. The thetas provided her are in the same order as the clusters in _nMembers.txt and they are drawn from the prior when they correspond to empty clusters.
_z.txt	This file includes the cluster membership for each observation at each sweep. Each row represents a sweep (including burn in if reportBurnIn=TRUE) and each element in the rows is the cluster membership for each of the observations,

There are more files that can be in the output, depending on which options are used in profRegr. The file \_mu.txt for example reports the mean for xModel=Normal, \_phi.txt reports the multinomial probabilities for xModel=Discrete, \_rho.txt reports the paramters for variable selection, etc. The files usually report one line for each sweep (including burn in if reportBurnIn=TRUE). See Liverani et al. (2015) for more details of the parameters.

ordered as they are provided to profRegr in the dataframe.

Note that for the \_gamma.txt for variable selection the results are reported per sweep (each line is a sweep) and within each line by cluster (so for each covariate the switches per cluster are reported in order, before the second covariate is reported for each cluster, etc).

#### **Authors**

David Hastie, Department of Epidemiology and Biostatistics, Imperial College London, UK

Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Aurore J. Lavigne, Department of Epidemiology and Biostatistics, Imperial College London, UK

Lamiae Azizi, MRC Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani diveranis@gmail.com>

The R package PReMiuM is supported through research grants. One key requirement of such funding applications is the ability to demonstrate the impact of the work we seek funding for can. Whatever you are using PReMiuM for, it would be very helpful for us to learn about our users, to tailor our future methodological developments to your needs. Please email us at liveranis@gmail.com or visit http://www.silvialiverani.com/support-premium/.

#### References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

Hastie, D. I., Liverani, S. and Richardson, S. (2014) Sampling from Dirichlet process mixture models with unknown concentration parameter: Mixing issues in large data implementations. *Forth-coming in the Statistics* & *Computing*. Available at http://link.springer.com/article/10.1007

setHyperparams 33

setHyperparams	Definition of characteristics of sample datasets for profile regression
setHyperparams	Definition of characteristics of sample datasets for profile regression

#### **Description**

Hyperparameters for the priors can be specified here and passed as an argument to profRegr.

The user can specify some or all hyperparameters. Those hyperparameters not specified will take their default values. Where the file is not provided, all hyperparameters will take their default values.

# Usage

#### **Arguments**

shapeAlpha	The shape parameter for Gamma prior on alpha (default=2)
rateAlpha	The inverse-scale (rate) parameter for the Gamma prior on alpha (default=1)
aPhi	The vector of parameters for the Dirichlet prior on phi_j. Element j corresponds to covariate j which then has a prior Dirichlet(aPhi[j],aPhi[j],,aPhi[j]). Only used in discrete case, default=(1 1 1 1).
mu0	The mean vector for mu_c in the Normal covariate case (only used in Normal covariate case, default=empirical covariate means)
Tau0	The precision matrix for mu_c in the Normal covariate case (only used in Normal covariate case, default=inverse of diagonal matrix with elements equal to squareof empirical range for each covariate)
RØ	The matrix parameter for the Wishart distribution for Tau_c (only used in Normal covariate case, default=1/nCovariates * inverse of empirical covariance matrix)
kappa0	The degrees of freedom parameter for the Wishart distribution for Tau_c (only used in Normal covariate case, default=nCovariates).
nu0	Hyperparameter for the conjugate Normal inverse Wishart prior for Normal covariates. The Normal distribution of mu_c has covariance Sigma_c/nu0. The default value is 0.01. The other hyperparameters for this parametrisation are reused from the independent priors. This hyperparameter is only useful when the option useNormInvWishPrior=TRUE in the function profRegr().
muTheta	The location parameter for the t-Distribution for theta_c (only used if response included in model, default=0)

34 setHyperparams

sigmaTheta The scale parameter for the t-Distribution for theta\_c (only used if response included in model, default=2.5) dofTheta The degrees of freedom parameter for the t-Distribution for theta\_c (only used if response included in model, default=7) muBeta The location parameter for the t-Distribution for beta (only used when fixed effects present, default=0) The scale parameter for the t-Distribution for beta (only used when fixed effects sigmaBeta present, default=2.5) dofBeta The dof parameter for the t-Distribution for beta (only used when fixed effects present, default=7) shapeTauEpsilon Shape parameter for gamma distribution for prior for precision tau of extra variation errors epsilon (only used if extra variation is used i.e. extraYVar argument is included, default=5.0) rateTauEpsilon Inverse-scale (rate) parameter for gamma distribution for prior for precision tau of extra variation errors epsilon (only used if extra variation is used i.e. extraY-Var argument is used, default=0.5) Parameter for beta distribution for prior on rho in variable selection (default=0.5) aRho bRho Parameter for beta distribution for prior on rho in variable selection (default=0.5) atomRho Parameter for the probability for the atom at zero, i.e. the 0.5 probability in w\_j distributed Bernoulli(0.5) in the formulation of the sparsity inducing prior (default=0.5). This parameter must be in the interval (0,1], where atomRho=1 corresponds to the case where the prior for rho is a Beta(aRho,bRho). shapeSigmaSqY Shape parameter of inverse-gamma prior for sigma\_Y^2 (only used in the Normal response model, default =2.5) scaleSigmaSqY Scale parameter of inverse-gamma prior for sigma\_Y^2 (only used in the Normal response model, default =2.5) pQuantile Quantile for the yModel=Quantile option (default = 0.5) Slice parameter for independent slice sampler such that  $xi_c = (1-rSlice)*rSlice^c$ rSlice for c=0,1,2,... (only used for slice independent sampler i.e. sampler=SliceIndependent, default 0.75). Parameter for determining the truncation level of the finite Dirichlet process truncationEps (only used for truncated sampler i.e. sampler=Truncated shapeTauCAR Shape parameter for gamma distribution for precision TauCAR of spatial CAR term (only used if a spatial term is included i.e. includeCAR argument is TRUE, default=0.001) Inverse-scale (rate) parameter for gamma distribution for precision TauCAR of rateTauCAR spatial CAR term (only used if a spatial term is included i.e. includeCAR argument is TRUE, default=0.001) shapeNu Shape parameter of Gamma prior for the shape parameter of the Weibull for survival response (only used in the Survival response model, default = 2.5) scaleNu Scale parameter of Gamma prior for the shape parameter of the Weibull for survival response (only used in the Survival response model, default = 1)

summarise VarSelectRho 35

initAlloc

Vector of the initial allocation of the individuals to clusters. This is NULL by default, which implies a random start. Useful for starting the MCMC from a specific partition. Note that if this overwrites the option nClusInit in the function profRegr: nClusInit is set equal to the maximum value in initAlloc.

#### Value

The output of this function is a list with the components defined as above.

#### **Authors**

David Hastie, Department of Epidemiology and Biostatistics, Imperial College London, UK

Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani liveranis@gmail.com>

#### References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

#### **Examples**

 $summarise Var Select Rho \quad summarise Var Select Rho \quad$ 

#### **Description**

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

# Usage

```
summariseVarSelectRho(runInfoObj)
```

36 summarise Var Select Rho

# **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.

#### **Authors**

David Hastie, Department of Epidemiology and Biostatistics, Imperial College London, UK

Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC

Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani liveranis@gmail.com>

#### References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

```
inputs <- generateSampleDataFile(clusSummaryVarSelectBernoulliDiscrete())
runInfoObj<-profRegr(yModel=inputs$yModel,
    xModel=inputs$xModel, nSweeps=10, nClusInit=15,
    nBurn=20, data=inputs$inputData, output="output",
    covNames = inputs$covNames, varSelect="Continuous")
rho<-summariseVarSelectRho(runInfoObj)</pre>
```

vec2mat 37

	nat

Vector to upper triangular matrix

# Description

Function to convert a vector to an upper triangular matrix. The vector does not include the diagonal values, which are then set equal to 1 in the matrix. The matrix is filled by row.

#### **Usage**

```
vec2mat(data = NA, nrow = 1)
```

# Arguments

data The vector to be converted, excluding the diagonal which is set equal to 1.

nrow The number of rows (and columns) of the resulting matrix.

#### Value

The symmetric matrix. The matrix is filled by column.

#### **Authors**

Silvia Liverani, Department of Epidemiology and Biostatistics, Imperial College London and MRC Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani diveranis@gmail.com>

# References

Silvia Liverani, David I. Hastie, Lamiae Azizi, Michail Papathomas, Sylvia Richardson (2015). PReMiuM: An R Package for Profile Regression Mixture Models Using Dirichlet Processes. Journal of Statistical Software, 64(7), 1-30. URL http://www.jstatsoft.org/v64/i07/.

```
vec2mat(data=c(1,2,3),nrow=3)
```

# **Index**

*Topic <b>hyperparameters</b>	clusSummaryCategoricalDiscrete
setHyperparams, 33	(clusSummaryBernoulliDiscrete),
*Topic margModelPosterior	13
margModelPosterior, 22	clusSummaryNormalDiscrete
*Topic <b>plots</b>	(clusSummaryBernoulliDiscrete),
plotRiskProfile, 24	13
*Topic <b>postprocessing</b>	clusSummaryNormalNormal
calcAvgRiskAndProfile,5	(clusSummaryBernoulliDiscrete),
calcDissimilarityMatrix,7	13
calcOptimalClustering, 8	clusSummaryNormalNormalSpatial
plotRiskProfile, 24	(clusSummaryBernoulliDiscrete),
*Topic <b>predictions</b> , <b>plots</b>	13
plotPredictions, 23	clusSummaryPoissonDiscrete
*Topic <b>predictions</b>	(clusSummaryBernoulliDiscrete),
calcPredictions, 9	13
*Topic <b>profileRegression</b>	clusSummaryPoissonNormal
profRegr, 26	(clusSummaryBernoulliDiscrete),
*Topic <b>simulation</b>	13
clusSummaryBernoulliDiscrete, 13	clusSummaryPoissonNormalSpatial
generateSampleDataFile, 16	(clusSummaryBernoulliDiscrete),
*Topic variableSelection	13
summariseVarSelectRho, 35	clusSummaryQuantileNormal
	(clusSummaryBernoulliDiscrete),
calcAvgRiskAndProfile, 5	13
calcDissimilarityMatrix,7	${\tt clusSummaryVarSelectBernoulliDiscrete}$
calcOptimalClustering, 8	(clusSummaryBernoulliDiscrete),
calcPredictions, 9	13
clusSummaryBernoulliDiscrete, 13	clusSummaryWeibullDiscrete
clusSummaryBernoulliDiscreteSmall	(clusSummaryBernoulliDiscrete),
$({\tt clusSummaryBernoulliDiscrete}),$	13
13	computeRatioOfVariance, 15
clusSummaryBernoulliMixed	
<pre>(clusSummaryBernoulliDiscrete),</pre>	generateSampleDataFile, 16
13	globalParsTrace, 17
clusSummaryBernoulliNormal	
<pre>(clusSummaryBernoulliDiscrete),</pre>	heatDissMat, 18
13	
clusSummaryBinomialNormal	is.wholenumber, 20
(clusSummaryBernoulliDiscrete),	
13	mapforGeneratedData, 21

INDEX 39

```
margModelPosterior, 22

plotPredictions, 23
plotRiskProfile, 24
PReMiuM (PReMiuM-package), 2
PReMiuM-package, 2
PReMiuMpackage (PReMiuM-package), 2
profRegr, 26

setHyperparams, 33
summariseVarSelectRho, 35

vec2mat, 37
```