

Package ‘PReMiuM’

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Type Package

Title Post processing for C++ PReMiuM

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Author David I. Hastie <david.hastie@rsimony.com>, Silvia Liverani <liveranis@gmail.com> and Sylvia Richardson <sylvia.richardson@mrc-bsu.cam.ac.uk>, with a contribution by Lamiae Azizi

Maintainer Silvia Liverani <liveranis@gmail.com>

Description Dirichlet process Bayesian Clustering, also known as profile regression.

License GPL (>= 3)

LazyLoad yes

Depends R (>= 2.15.2), Rcpp (>= 0.9.15), cluster (>= 1.14.3), ggplot2 (>= 0.9.2.1), grid, clue (>= 0.3-45)

LinkingTo Rcpp

SystemRequirements GNU make

R topics documented:

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| | |
|-----------------|--|
| PReMiuM-package | <i>Dirichlet Process Bayesian Clustering</i> |
|-----------------|--|

Description

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

Details

| | |
|-----------|------------|
| Package: | PReMiuM |
| Type: | Package |
| Version: | 3.0.4 |
| Date: | 2013-01-10 |
| License: | GPL3 |
| LazyLoad: | yes |

Program to implement Dirichlet Process Bayesian Clustering as described in Liverani et al. 2013. Previously this project was called profile regression.

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 or Normal responses
- Handles inclusion of fixed effects in the response model
- 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 is 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

Maintainer: Silvia Liverani <liveranis@gmail.com>

Acknowledgements

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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., 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. *Submitted*.

Molitor, J., Brown, I. J., Papathomas, M., Molitor, N., Liverani, S., Chan, Q., Richardson, S., Van Horn, L., Daviglius, M. L., Stamler, J. and Elliott, P. (2013) Blood pressure differences associated with DASH-like lower sodium compared with typical American higher sodium nutrient profile: INTERMAP USA. *Submitted*.

Hastie, D. I., Liverani, S. and Richardson, S. (2013) Sampling from Dirichlet process mixture models with unknown concentration parameter. *Submitted*.

Liverani, S., Hastie, D. I. and Richardson, S. (2013) PReMiuM: An R package for Profile Regression Mixture Models using Dirichlet Processes. *Submitted*.

Examples

```
# example for Poisson outcome and Discrete covariates
inputs <- generateSampleDataFile(clusSummaryPoissonDiscrete())
runInfoObj<-profRegr(yModel=inputs$yModel,
  xModel=inputs$xModel, nSweeps=10, nClusInit=20,
  nBurn=20, data=inputs$inputData, output="output",
```

```

covNames = inputs$covNames, outcomeT = inputs$outcomeT,
fixedEffectsNames = inputs$fixedEffectNames)

dissimObj<-calcDissimilarityMatrix(runInfoObj)
clusObj<-calcOptimalClustering(dissimObj)
riskProfileObj<-calcAvgRiskAndProfile(clusObj)
clusterOrderObj<-plotRiskProfile(riskProfileObj,"summary.png")

```

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. 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. |

Value

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

| | |
|-----------------|--|
| riskProfClusObj | 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. |
| profile | 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 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 exist 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 number 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. |

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

Liverani, S., Hastie, D. I. and Richardson, S. (2013) PReMiuM: An R package for Profile Regression Mixture Models using Dirichlet Processes. *Submitted*.

Examples

```
generateDataList <- clusSummaryBernoulliDiscrete()
inputs <- generateSampleDataFile(generateDataList)
runInfoObj<-profRegr(yModel=inputs$yModel, xModel=inputs$xModel, nSweeps=10,
  nBurn=20, data=inputs$inputData, output="output", nClusInit=15,
  covNames=inputs$covNames)

dissimObj<-calcDissimilarityMatrix(runInfoObj)
clusObj<-calcOptimalClustering(dissimObj)
riskProfileObj<-calcAvgRiskAndProfile(clusObj)
```

calcDissimilarityMatrix

Calculates the dissimilarity matrix

Description

Calculates the dissimilarity matrix.

Usage

```
calcDissimilarityMatrix(runInfoObj)
```

Arguments

runInfoObj 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 contains the upper triangle diagonal entries.

disSimMatPred

The dissimilarity matrix, again in vector format as above, for the predicted subjects.

lsOptSweep

The optimal partition among those explored by the MCMC, as defined by the least squares method. See Dahl (2006).

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

Liverani, S., Hastie, D. I. and Richardson, S. (2013) PReMiuM: An R package for Profile Regression Mixture Models using Dirichlet Processes. *Submitted*.

Examples

```
generateDataList <- clusSummaryBernoulliDiscrete()
inputs <- generateSampleDataFile(generateDataList)
runInfoObj<-profRegr(yModel=inputs$yModel, xModel=inputs$xModel,
  nSweeps=10, nBurn=20, data=inputs$inputData, output="output",
  covNames=inputs$covNames,nClusInit=15)

dissimObj<-calcDissimilarityMatrix(runInfoObj)
```

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 calcDissimilarityMatrix(), and as described in ?calcDissimilarityMatrix) or a list of dissimilarity 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 number 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. 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
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References

Liverani, S., Hastie, D. I. and Richardson, S. (2013) PReMiuM: An R package for Profile Regression Mixture Models using Dirichlet Processes. *Submitted*.

Examples

```
generateDataList <- clusSummaryBernoulliDiscrete()
inputs <- generateSampleDataFile(generateDataList)
runInfoObj<-profRegr(yModel=inputs$yModel, xModel=inputs$xModel,
  nSweeps=10, nBurn=20, data=inputs$inputData, output="output",
  covNames=inputs$covNames, nClusInit=15)

dissimObj<-calcDissimilarityMatrix(runInfoObj)
clusObj<-calcOptimalClustering(dissimObj)
```

| | |
|-----------------|-----------------------------------|
| calcPredictions | <i>Calculates the predictions</i> |
|-----------------|-----------------------------------|

Description

Calculates the predictions.

Usage

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

Arguments

| | |
|-------------------------|--|
| riskProfObj | Object of type riskProfObj. |
| predictResponseFileName | The file which contains the predictive scenarios, as it is produced by the code and stored. |
| 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. |

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. |
| observedY | The values of the outcome provided by the user. This is in the case that predictions 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 mean 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 otherwise. |
| 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). |

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.

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

Liverani, S., Hastie, D. I. and Richardson, S. (2013) PReMiuM: An R package for Profile Regression Mixture Models using Dirichlet Processes. *Submitted*.

Examples

```
inputs <- generateSampleDataFile(clusSummaryBernoulliDiscrete())

# prediction profiles
preds<-data.frame(matrix(c(0, 0, 1, 0, 0,
0, 0, 1, NA, 0),ncol=5,byrow=TRUE))
colnames(preds)<-names(inputs$inputData)[2:(inputs$nCovariates+1)]

# run profile regression
runInfoObj<-profRegr(yModel=inputs$yModel, xModel=inputs$xModel,
  nSweeps=100, nBurn=1000, data=inputs$inputData, output="output",
  covNames=inputs$covNames,predict=preds)

# postprocessing
dissimObj <- calcDissimilarityMatrix(runInfoObj)
clusObj <- calcOptimalClustering(dissimObj)
riskProfileObj <- calcAvgRiskAndProfile(clusObj)
clusterOrderObj <- plotRiskProfile(riskProfileObj,"summary.png",
  whichCovariates=c(1,2))
output_predictions <- calcPredictions(riskProfileObj,fullSweepPredictions=TRUE)

# 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())

# 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)]

# run profile regression
runInfoObj<-profRegr(yModel=inputs$yModel,
  xModel=inputs$xModel, nSweeps=100,
  nBurn=100, data=inputs$inputData, output="output",
  covNames = inputs$covNames, outcomeT="outcomeT",
  fixedEffectsNames = inputs$fixedEffectNames,predict=predsPoisson)

# postprocessing
```

```

dissimObj<-calcDissimilarityMatrix(runInfoObj)
clusObj<-calcOptimalClustering(dissimObj)
riskProfileObj<-calcAvgRiskAndProfile(clusObj)
output_predictions <- calcPredictions(riskProfileObj,fullSweepPredictions=TRUE)

# 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())

# 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)]

# run profile regression
runInfoObj<-profRegr(yModel=inputs$yModel,
    xModel=inputs$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)
clusObj<-calcOptimalClustering(dissimObj)
riskProfileObj<-calcAvgRiskAndProfile(clusObj)
output_predictions <- calcPredictions(riskProfileObj,fullSweepPredictions=TRUE)

```

clusSummaryBernoulliDiscrete

Sample datasets for profile regression

Description

Definition of skeleton of sample datasets for profile regression.

Usage

```

clusSummaryBernoulliDiscrete()
clusSummaryBinomialNormal()
clusSummaryCategoricalDiscrete()
clusSummaryNormalDiscrete()
clusSummaryNormalNormal()
clusSummaryPoissonDiscrete()

```

```
clusSummaryPoissonNormal()
clusSummaryVarSelectBernoulliDiscrete()
clusSummaryBernoulliMixed()
```

Value

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

| | |
|---------------------------------|---|
| <code>outcomeType</code> | The outcome type of the dataset. |
| <code>covariateType</code> | The covariate type of the dataset. |
| <code>nCovariates</code> | The number of covariates generated. |
| <code>nCategories</code> | The number of categories of the covariates if the covariates are discrete or mixed. |
| <code>nFixedEffects</code> | The number of fixed effects. |
| <code>fixedEffectsCoeffs</code> | The names of the fixed effects. |
| <code>missingDataProb</code> | The pobability of generating missing data. |
| <code>nClusters</code> | The number of clusters. |
| <code>clusterSizes</code> | The number of observations in each cluster. |
| <code>clusterData</code> | The dataset, including the outcome, the covariates, the fixed effects, the number of trials (if Binomial outcome) and the offset (for Poisson outcome). |
| <code>covNames</code> | The names of the covariates of the dataset. |
| <code>nDiscreteCovs</code> | The number of discrete covariates, if the covariate type is mixed. |
| <code>nContinuousCovs</code> | The number of continuous covariates, if the covariate type is mixed. |
| <code>outcomeT</code> | The name of the column of the dataset containing the number of trials (if Binomial outcome) or the offset (for Poisson outcome). |

Details

`clusSummaryBernoulliDiscrete` generates a dataset with Bernoulli outcome and discrete covariates.
`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.

`clusSummaryPoissonDiscrete` generates a dataset with Poisson outcome and discrete covariates.

`clusSummaryPoissonNormal` generates a dataset with Poisson outcome and Normal covariates.

`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.

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

Liverani, S., Hastie, D. I. and Richardson, S. (2013) PReMiuM: An R package for Profile Regression Mixture Models using Dirichlet Processes. *Submitted*.

Examples

```
clusSummaryBernoulliDiscrete()
```

```
generateSampleDataFile
```

Generate sample data files for profile regression

Description

Generation of random sample datasets for profile regression.

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

| | |
|-------------------------------|---|
| <code>yModel</code> | The outcome model according to which the data has been generated. |
| <code>xModel</code> | The covariate model according to which the data has been generated. |
| <code>inputData</code> | The data.frame that contains the data. |
| <code>covNames</code> | The names of the covariates. |
| <code>fixedEffectNames</code> | The names of the fixed effects. |

Authors

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

Liverani, S., Hastie, D. I. and Richardson, S. (2013) PReMiuM: An R package for Profile Regression Mixture Models using Dirichlet Processes. *Submitted*.

Examples

```
# generation of data for clustering

generateDataList <- clusSummaryBernoulliDiscrete()
inputs <- generateSampleDataFile(generateDataList)
```

| | |
|----------------|--|
| is.wholenumber | <i>Function to check if a number is a whole number</i> |
|----------------|--|

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.

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

Liverani, S., Hastie, D. I. and Richardson, S. (2013) PReMiuM: An R package for Profile Regression Mixture Models using Dirichlet Processes. *Submitted*.

Examples

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

| | |
|--------------------|---------------------------------|
| margModelPosterior | <i>Marginal Model Posterior</i> |
|--------------------|---------------------------------|

Description

Compute the marginal model posterior.

Usage

```
margModelPosterior(runInfoObj)
```

Arguments

runInfoObj An object of type runInfoObj.

Value

It returns a file in the output folder, with name ending in "_margModPost.txt", that contains the marginal model posterior. It also returns the mean of the values of the marginal model posterior as they appear in the file ending in "_margModPost.txt" in the output folder.

Authors

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

Maintainer: Silvia Liverani <liveranis@gmail.com>

References

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Examples

```
inputs <- generateSampleDataFile(clusSummaryBernoulliDiscrete())

runInfoObj<-profRegr(yModel=inputs$yModel,
  xModel=inputs$xModel, nSweeps=5,
  nBurn=10, data=inputs$inputData, output="output",
  covNames = inputs$covNames, nClusInit=15,
  fixedEffectsNames = inputs$fixedEffectNames)

margModelPosterior(runInfoObj)
```

| | |
|-----------------|-------------------------------|
| plotRiskProfile | <i>Plot the Risk Profiles</i> |
|-----------------|-------------------------------|

Description

Plots the risk profiles for a profile regression model.

Usage

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

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. |
| 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 indices 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 indices 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. |

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 $\sqrt{\text{Sigma}[j,j]}$ (i.e. the standard deviation for that covariate).

It also returns the following vector.

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

Liverani, S., Hastie, D. I. and Richardson, S. (2013) PReMiuM: An R package for Profile Regression Mixture Models using Dirichlet Processes. *Submitted*.

Examples

```
# example for Poisson outcome and Discrete covariates
inputs <- generateSampleDataFile(clusSummaryPoissonDiscrete())
runInfoObj<-profRegr(yModel=inputs$yModel,
  xModel=inputs$xModel, nSweeps=10, nClusInit=15,
  nBurn=20, data=inputs$inputData, output="output",
  covNames = inputs$covNames, outcomeT = inputs$outcomeT,
  fixedEffectsNames = inputs$fixedEffectNames)

dissimObj<-calcDissimilarityMatrix(runInfoObj)
clusObj<-calcOptimalClustering(dissimObj)
riskProfileObj<-calcAvgRiskAndProfile(clusObj)
clusterOrderObj<-plotRiskProfile(riskProfileObj,"summary.png")
```

Description

Fit a profile regression model.

Usage

```
profRegr(covNames, fixedEffectsNames, outcome="outcome",
         outcomeT=NA, data, output="output", hyper, predict,
         nSweeps=1000, nBurn=1000, nProgress=500, nFilter=1,
         nClusInit, seed, yModel="Bernoulli", xModel="Discrete",
         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 | Object of type setHyperparams with hyperparameters specifications. This is optional, default values are provided for all hyperparameters. See ?setHyperparams for details. |
| predict | <p>Data frame containing the predictive scenarios. This is only required if predictions are requested.</p> <p>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).</p> <p>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 processing function calcPredictions will create predicted response values for these subjects.</p> <p>See ?calcPredictions for more details and examples.</p> |

| | |
|----------------|--|
| 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 "Discrete", "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 default the extra Gaussian variance is not included. |
| varSelectType | The type of variable selection to be used "None", "BinaryCluster" or "Continuous". The default value is "None". |
| entropy | If included then we compute allocation entropy. By default the allocation entropy 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

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`.

| | |
|-------------------------------|---|
| <code>directoryPath</code> | String. Directory path of the output files. |
| <code>fileStem</code> | String. The |
| <code>inputFileName</code> | String. Location and file name of input dataset as created by this function for the C++ routines |
| <code>nSweeps</code> | Integer. The number of sweeps of the MCMC after the burn-in. |
| <code>nBurn</code> | Integer. The number of iterations in the burn-in period of the MCMC. |
| <code>reportBurnIn</code> | Logical. Whether the output of the burn-in report should be included. |
| <code>nFilter</code> | Integer. The frequency (in sweeps) with which to write the output to file. The default value is 1. |
| <code>nSubjects</code> | Integer. The number of subjects. |
| <code>nPredictSubjects</code> | Integer. The number of subjects for which to run predictions. |
| <code>covNames</code> | A vector of strings with the names of the covariates. |
| <code>xModel</code> | String. The model type for the covariates. |
| <code>includeResponse</code> | Logical. If FALSE only the covariate data X is modelled. |
| <code>yModel</code> | String. The model type for the outcome. |
| <code>varSelect</code> | Logical. If FALSE no variable selection is performed. |
| <code>varSelectType</code> | String. It specifies what type of variable selection has been performed, if any. |
| <code>nCovariates</code> | Integer. The number of covariates. |
| <code>nFixedEffects</code> | Integer. The number of fixed effects. |
| <code>nCategoriesY</code> | Integer. The number of categories of the outcome, if <code>yModel = "Categorical"</code> . It is 1 otherwise. |
| <code>nCategories</code> | Vector of integers. The number of categories of each covariate, if <code>xModel = "Discrete"</code> . It is 1 otherwise. |
| <code>xMat</code> | A matrix of the covariate data. |
| <code>yMat</code> | A matrix of the outcome data, including the offset if the outcome is Poisson and the number of trials if the outcome is Binomial. |
| <code>wMat</code> | A matrix of the fixed effect data. |

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

and a contribution for mixed covariates by Lamiae Azizi, MRC Biostatistics Unit, Cambridge, UK

Maintainer: Silvia Liverani <liveranis@gmail.com>

References

Liverani, S., Hastie, D. I. and Richardson, S. (2013) PReMiuM: An R package for Profile Regression Mixture Models using Dirichlet Processes. *Submitted*.

Examples

```
# example for Poisson outcome and Discrete covariates
inputs <- generateSampleDataFile(clusSummaryPoissonDiscrete())
runInfoObj<-profRegr(yModel=inputs$yModel,
  xModel=inputs$xModel, nSweeps=10, nClusInit=20,
  nBurn=20, data=inputs$inputData, output="output",
  covNames = inputs$covNames, outcomeT = inputs$outcomeT,
  fixedEffectsNames = inputs$fixedEffectNames)

# example with Bernoulli outcome and Mixed covariates
inputs <- generateSampleDataFile(clusSummaryBernoulliMixed())
runInfoObj<-profRegr(yModel=inputs$yModel,
  xModel=inputs$xModel, nSweeps=10, nClusInit=15,
  nBurn=20, data=inputs$inputData, output="output",
  discreteCovs = inputs$discreteCovs,
  continuousCovs = inputs$continuousCovs)
```

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

```
setHyperparams(shapeAlpha=NULL, rateAlpha=NULL,
  useReciprocalNCatsPhi=NULL, aPhi=NULL, mu0=NULL, Tau0=NULL, R0=NULL,
  kapp0=NULL, muTheta=NULL, sigmaTheta=NULL, dofTheta=NULL, muBeta=NULL,
  sigmaBeta=NULL, dofBeta=NULL, shapeTauEpsilon=NULL,
  rateTauEpsilon=NULL, aRho=NULL, bRho=NULL, shapeSigmaSqY=NULL,
  scaleSigmaSqY=NULL, rSlice=NULL, truncationEps=NULL)
```

Arguments

| | |
|------------|---|
| shapeAlpha | The shape parameter for Gamma prior on alpha (default=1.0) |
| rateAlpha | The inverse-scale (rate) parameter for the Gamma prior on alpha (default=0.5) |

| | |
|-----------------------|--|
| useReciprocalNCatsPhi | Boolean denoting whether the vector ϕ_j (for covariate j) have all elements equal (only used in the discrete covariate case, default=true) |
| aPhi | The vector of parameters for the Dirichlet prior on ϕ_j . Element j corresponds to covariate j which then has a prior $\text{Dirichlet}(a\phi[j], a\phi[j], \dots, a\phi[j])$. (Only used in discrete case if useReciprocalNCatsPhi is false, default=(1 1 1 ... 1)) |
| mu0 | The mean vector for μ_c in the Normal covariate case (only used in Normal covariate case, default=empirical covariate means) |
| Tau0 | The precision matrix for μ_c in the Normal covariate case (only used in Normal covariate case, default=inverse of diagonal matrix with elements equal to square of empirical range for each covariate) |
| R0 | The matrix parameter for the Wishart distribution for τ_c (only used in Normal covariate case, default= $1/n\text{Covariates} * \text{inverse of empirical covariance matrix}$) |
| kapp0 | The degrees of freedom parameter for the Wishart distribution for τ_c (only used in Normal covariate case, default= $n\text{Covariates}$). |
| muTheta | The location parameter for the t-Distribution for θ_c (only used if response included in model, default=0) |
| sigmaTheta | The scale parameter for the t-Distribution for θ_c (only used if response included in model, default=2.5) |
| dofTheta | The degrees of freedom parameter for the t-Distribution for θ_c (only used if response included in model, default=7) |
| muBeta | The location parameter for the t-Distribution for β (only used when fixed effects present, default=0) |
| sigmaBeta | The scale parameter for the t-Distribution for β (only used when fixed effects present, default=2.5) |
| dofBeta | The dof parameter for the t-Distribution for β (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. extraYVar argument is used, default=0.5) |
| aRho | Parameter for beta distribution for prior on rho in variable selection (default=0.5) |
| bRho | Parameter for beta distribution for prior on rho in variable selection (default=0.5) |
| shapeSigmaSqY | Shape parameter of inverse-gamma prior for σ_Y^2 (only used in the Normal response model, default =2.5) |
| scaleSigmaSqY | Scale parameter of inverse-gamma prior for σ_Y^2 (only used in the Normal response model, default =2.5) |
| rSlice | Slice parameter for independent slice sampler such that $x_{i,c} = (1-r\text{Slice}) * r\text{Slice}^c$ for $c=0,1,2,\dots$ (only used for slice independent sampler i.e. sampler=SliceIndependent, default 0.75). |

truncationEps Parameter for determining the truncation level of the finite Dirichlet process (only used for truncated sampler i.e. sampler=Truncated)

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

Liverani, S., Hastie, D. I. and Richardson, S. (2013) PReMiuM: An R package for Profile Regression Mixture Models using Dirichlet Processes. *Submitted*.

Examples

```
hyp <- setHyperparams(shapeAlpha=3,rateAlpha=2,mu0=c(30,13),R0=3.2*diag(2))

inputs <- generateSampleDataFile(clusSummaryPoissonNormal())
runInfoObj<-profRegr(yModel=inputs$yModel,
  xModel=inputs$xModel, nSweeps=2, nClusInit=15,
  nBurn=2, data=inputs$inputData, output="output",
  covNames = inputs$covNames, outcomeT = inputs$outcomeT,
  fixedEffectsNames = inputs$fixedEffectNames,
  hyper=hyp)
```

summariseVarSelectRho *summariseVarSelectRho*

Description

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

Usage

```
summariseVarSelectRho(runInfoObj)
```

Arguments

runInfoObj 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 posterior 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 corresponds 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

Liverani, S., Hastie, D. I. and Richardson, S. (2013) PReMiuM: An R package for Profile Regression Mixture Models using Dirichlet Processes. *Submitted*.

Examples

```
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)
```


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