Package: AdaptGauss (via r-universe)

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Type Package

```
Title Gaussian Mixture Models (GMM)
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Maintainer Michael Thrun <m. thrun@gmx.net>
Description Multimodal distributions can be modelled as a mixture of
     components. The model is derived using the Pareto Density
     Estimation (PDE) for an estimation of the pdf. PDE has been
     designed in particular to identify groups/classes in a dataset.
     Precise limits for the classes can be calculated using the
     theorem of Bayes. Verification of the model is possible by QQ
     plot, Chi-squared test and Kolmogorov-Smirnov test. The package
     is based on the publication of Ultsch, A., Thrun, M.C.,
     Hansen-Goos, O., Lotsch, J. (2015) < DOI:10.3390/ijms161025897>.
Imports Rcpp, shiny, pracma, methods, DataVisualizations
Suggests mclust, grid, foreach, dqrng, parallelDist, knitr (>= 1.12),
     rmarkdown (>= 0.9), reshape2, ggplot2, plotly
LinkingTo Rcpp
Depends R (>= 2.10)
License GPL-3
LazyLoad yes
URL https://www.uni-marburg.de/fb12/datenbionik/software-en
Encoding UTF-8
NeedsCompilation yes
VignetteBuilder knitr
BugReports https://github.com/Mthrun/AdaptGauss/issuesConfig/pak/sysreqs:
     make libicu-dev zlib1g-dev
Repository https://mthrun.r-universe.dev
RemoteUrl https://github.com/mthrun/adaptgauss
RemoteRef HEAD
RemoteSha d0a5d20d90eb51faf41af16c01a507d6e41d9416
```

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Adap [*]	tGauss-package Gaussian Mixture Models (GMM)	

Description

Multimodal distributions can be modelled as a mixture of components. The model is derived using the Pareto Density Estimation (PDE) for an estimation of the pdf. PDE has been designed in particular to identify groups/classes in a dataset. Precise limits for the classes can be calculated using the theorem of Bayes. Verification of the model is possible by QQ plot, Chi-squared test and Kolmogorov-Smirnov test. The package is based on the publication of Ultsch, A., Thrun, M.C., Hansen-Goos, O., Lotsch, J. (2015) <DOI:10.3390/ijms161025897>.

Details

Multimodal distributions can be modelled as a mixture of components. The model is derived using the Pareto Density Estimation (PDE) for an estimation of the pdf [Ultsch 2005]. PDE has been designed in particular to identify groups/classes in a dataset. The expectation maximization algorithm estimates a Gaussian mixture model of density states [Bishop 2006] and the limits between the different states are defined by Bayes decision boundaries [Duda 2001]. The model can be verified with Chi-squared test, Kolmogorov-Smirnov test and QQ plot.

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The correct number of modes may be found with AIC or BIC.

Index: This package was not yet installed at build time.

Author(s)

Michael Thrun, Onno Hansen-Goos, Rabea Griese, Catharina Lippmann, Florian Lerch, Jorn Lotsch, Alfred Ultsch Maintainer: Michael Thrun <m.thrun@gmx.net>

References

Ultsch, A., Thrun, M.C., Hansen-Goos, O., Loetsch, J.: Identification of Molecular Fingerprints in Human Heat Pain Thresholds by Use of an Interactive Mixture Model R Toolbox(AdaptGauss), International Journal of Molecular Sciences, doi:10.3390/ijms161025897, 2015.

Duda, R.O., P.E. Hart, and D.G. Stork, Pattern classification. 2nd. Edition. New York, 2001, p 512 ff

Bishop, Christopher M. Pattern recognition and machine learning. springer, 2006, p 435 ff

Ultsch, A.: Pareto density estimation: A density estimation for knowledge discovery, in Baier, D.; Werrnecke, K. D., (Eds), Innovations in classification, data science, and information systems, Proc Gfkl 2003, pp 91-100, Springer, Berlin, 2005.

Thrun M.C., Ultsch, A.: Models of Income Distributions for Knowledge Discovery, European Conference on Data Analysis, DOI 10.13140/RG.2.1.4463.0244, Colchester 2015.

Examples

```
## Statistically significant GMM

data=c(rnorm(3000,2,1),rnorm(3000,7,3),rnorm(3000,-2,0.5))
gmm=AdaptGauss::AdaptGauss(data,

Means = c(-2, 2, 7),

SDs = c(0.5, 1, 4),

Weights = c(0.3333, 0.3333, 0.3333))

AdaptGauss::Chi2testMixtures(data,
gmm$Means,gmm$SDs,gmm$Weights,PlotIt=T)

AdaptGauss::QQplotGMM(data,gmm$Means,gmm$SDs,gmm$Weights)

## Statistically non significant GMM

data('LKWFahrzeitSeehafen2010')
gmm=AdaptGauss::AdaptGauss(LKWFahrzeitSeehafen2010,
```

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```
Means = c(52.74, 385.38, 619.46, 162.08),
SDs = c(38.22, 93.21, 57.72, 48.36),
Weights = c(0.2434, 0.5589, 0.1484, 0.0749))
AdaptGauss::Chi2testMixtures(LKWFahrzeitSeehafen2010,
gmm$Means,gmm$SDs,gmm$Weights,PlotIt=T)
AdaptGauss::QQplotGMM(LKWFahrzeitSeehafen2010,gmm$Means,gmm$SDs,gmm$Weights)
```

AdaptGauss

Adapt Gaussian Mixture Model (GMM)

Description

Adapt interactively a Gaussians Mixture Model GMM to the empirical PDF of the data (generated by DataVisualizations::ParetoDensityEstimation) such that N(Means,SDs)*Weights is a model for Data

Usage

```
AdaptGauss(Data, Means = NaN, SDs = NaN, Weights = NaN,

ParetoRadius = NaN, LB = NaN, HB = NaN,

ListOfAdaptGauss, fast = T)
```

Arguments

Data	Data for empirical PDF. Has to be an Array of values. NaNs and NULLs will be deleted
Means	Optional: Means of gaussians of GMM.
SDs	Optional: StandardDevations of gaussians of GMM. (Has to be the same length as Means)
Weights	Optional: Weights of gaussians of GMM. (Has to be the same length as Means)
ParetoRadius	Optional: Pareto Radius of Pareto Desity Estimation (PDE).
LB	Optional: Low boundary of estimation. All values below LB will be deleted. Default: min(Data)
НВ	Optional: High boundary of estimation. All values above HB will be deleted. Default: max(Data)

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ListOfAdaptGauss

Optional: If editing of an existing Model is the goal, enables to give the Output of AdaptGaus as the Input of AdaptGauss() instead of setting Means, SDs and

Weights separately

fast Default=TRUE; FALSE: Using mclust's EM see function densityMclust of

that package, TRUE: Naive but faster EM implementation, which may be nu-

merical unstable, because log(gauss) is not used

Details

Data: maximum length is 10000. If larger, Data will be randomly reduced to 10000 Elements. MeansIn/DeviationsIn/WeightsIN: If empty, either one or three Gaussian's are generated by kmeans algorithm. Pareto Radius: If empty: will be generated by DataVisualizations::ParetoDensityEstimation RMS: Root Mean Square error is normalized by RMS of Gaussian's with Mean=mean(data) and SD=sd(data), see [Ultsch et.al., 2015] for further details.

Value

List with

Means of Gaussian's.

SDs Standard SDs of Gaussian's.

Weights Weights of Gaussian's.

ParetoRadius Pareto Radius: Either ParetoRadiusIn, the pareto radius enerated by PretoDen-

sityEstimation(if no Pareto Radius in Input).

RMS Root Mean Square of Deviation between Gaussian Mixture Model GMM to the

empirical PDF. Normalized by RMS of one Gaussian with mean=meanrobust(data)

and sdev=stdrobust(data). Further Details in [Ultsch et al 2015]

BayesBoundaries

vector[1:L-1], Bayes decision boundaries

Author(s)

Onno Hansen-Goos, Michael Thrun

References

Ultsch, A., Thrun, M.C., Hansen-Goos, O., Loetsch, J.: Identification of Molecular Fingerprints in Human Heat Pain Thresholds by Use of an Interactive Mixture Model R Toolbox(AdaptGauss), International Journal of Molecular Sciences, doi:10.3390/ijms161025897, 2015.

Thrun M.C., Ultsch, A.: Models of Income Distributions for Knowledge Discovery, European Conference on Data Analysis, DOI 10.13140/RG.2.1.4463.0244, Colchester 2015.

Examples

data1=c(rnorm(1000))

Not run: Vals1=AdaptGauss(data1)

Bayes4Mixtures

```
 \begin{array}{l} {\tt data2=c(rnorm(1000),rnorm(2000)+2,rnorm(1000)*2-1)} \\ {\tt \#\# Not\ run:\ Vals2=AdaptGauss(data2,c(-1,0,2),c(2,1,1),c(0.25,0.25,0.5),0.3,-6,6)} \\ \end{array}
```

Bayes4Mixtures

Posterioris of Bayes Theorem

Description

Calculates the posterioris of Bayes theorem

Usage

```
Bayes4Mixtures(Data, Means, SDs, Weights, IsLogDistribution,
PlotIt, CorrectBorders, Color, xlab, lwd)
```

Arguments

Data	vector (1:N) of data points
Means	vector[1:L] of Means of Gaussians (of GMM),L == Number of Gaussians
SDs	vector of standard deviations, estimated Gaussian Kernels, has to be the same length as Means
Weights	vector of relative number of points in Gaussians (prior probabilities), has to be the same length as Means
IsLogDistribut	ion
	Optional, ==1 if distribution(i) is a LogNormal, default vector of zeros of length L
PlotIt	Optional, Default: FALSE; TRUE do a Plot
CorrectBorders	Optional, ==TRUE data at right borders of GMM distribution will be assigned to last gaussian, left border vice versa. (default ==FALSE) normal Bayes Theorem
Color	Optional, character vector of colors, default rainbow()
xlab	

Width of Line, see intern R documentation

Details

lwd

See conference presentation for further explanation.

Value

List with

Posteriors (1:N,1:L) of Posteriors corresponding to Data

NormalizationFactor

(1:N) denominator of Bayes theorem corresponding to Data

BayesClassification 7

Author(s)

Catharina Lippmann, Onno Hansen-Goos, Michael Thrun

References

Thrun M.C., Ultsch, A.: Models of Income Distributions for Knowledge Discovery, European Conference on Data Analysis, DOI 10.13140/RG.2.1.4463.0244, Colchester 2015.

See Also

 ${\tt BayesDecisionBoundaries,} {\tt AdaptGauss}$

 $Bayes Classification \qquad \textit{Bayes Classification}$

Description

Bayes Klassifikation den Daten zuordnen

Usage

```
BayesClassification(Data, Means, SDs, Weights, IsLogDistribution = Means
  * 0, ClassLabels = c(1:length(Means)))
```

Arguments

Data	vector of Data
Means	vector[1:L] of Means of Gaussians (of GMM)
SDs	vector of standard deviations, estimated Gaussian Kernels, has to be the same length as Means
Weights	vector of relative number of points in Gaussians (prior probabilities), has to be the same length as Means
IsLogDistributi	on
	Optional, ==1 if distribution(i) is a LogNormal, default vector of zeros of length 1:L
ClassLabels	Optional numbered class labels that are assigned to the classes. default (1:L), L

Value

Cls(1:n,1:d) classiffication of Data, such that 1= first component of gaussian mixture model, 2= second component of gaussian mixture model and so on. For Every datapoint a number is returned.

number of different components of gaussian mixture model

Author(s)

Michael Thrun

BayesDecisionBoundaries

Decision Boundaries calculated through Bayes Theorem

Description

Function finds the intersections of Gaussians or LogNormals

Usage

BayesDecisionBoundaries(Means,SDs,Weights,IsLogDistribution,MinData,MaxData,Ycoor)

Arguments

Means vector[1:L] of Means of Gaussians (of GMM)

SDs vector of standard deviations, estimated Gaussian Kernels, has to be the same

length as Means

Weights vector of relative number of points in Gaussians (prior probabilities), has to be

the same length as Means

 ${\tt IsLogDistribution}$

Optional, ==1 if distribution(i) is a LogNormal, default vector of zeros of length

1:L

MinData Optional, Beginning of range, where the Boundaries are searched for, default

min(M)

MaxData Optional, End of range, where the Boundaries are searched for, default max(M) Ycoor Optional, Bool, if TRUE instead of vector of DecisionBoundaries list of DecisionBoundaries

sionBoundaries and DBY is returned

Value

DecisionBoundaries

vector[1:L-1], Bayes decision boundaries

DBY if (Ycoor==TRUE), y values at the cross points of the Gaussians is also returned,

that the return is a list of DecisionBoundaries and DBY

Author(s)

Michael Thrun, Rabea Griese

References

Duda, R. O., Hart, P. E., & Stork, D. G. (2001). Pattern classification. 2nd. Edition. New York, p. 512ff

See Also

 $Adapt Gauss, Intersect 2 \verb|Mixtures|, Bayes 4 \verb|Mixtures|$

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BayesFor2GMM Posterioris of Bayes Theorem for a two group GMM	
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Description

Calculates the posterioris of Bayes theorem, splits the GMM in two groups beforehand.

Usage

```
BayesFor2GMM(Data, Means, SDs, Weights, IsLogDistribution = Means * 0,
   Ind1 = c(1:floor(length(Means)/2)), Ind2 = c((floor(length(Means)/2)
   + 1):length(Means)), PlotIt = 0, CorrectBorders = 0)
```

Arguments

Data	vector (1:N) of data points
Means	vector[1:L] of Means of Gaussians (of GMM),L == Number of Gaussians
SDs	vector of standard deviations, estimated Gaussian Kernels, has to be the same length as Means
Weights	vector of relative number of points in Gaussians (prior probabilities), has to be the same length as Means
IsLogDistribut	ion
	Optional, ==1 if distribution(i) is a LogNormal, default vector of zeros of length L
Ind1	indices from (1:C) such that $[M(Ind1),S(Ind1),W(Ind1)]$ is one mixture, $[M(Ind2),S(Ind2),W(Ind2)]$ the second mixture default $Ind1=1:C/2,Ind2=C/2+1:C$
Ind2	indices from (1:C) such that $[M(Ind1),S(Ind1),W(Ind1)]$ is one mixture, $[M(Ind2),S(Ind2),W(Ind2)]$ the second mixture default $Ind1=1:C/2$, $Ind2=C/2+1:C$
PlotIt	Optional, Default: FALSE; TRUE do a Plot
CorrectBorders	Optional, ==TRUE data at right borders of GMM distribution will be assigned to last gaussian, left border vice versa. (default ==FALSE) normal Bayes Theorem

Details

See conference presentation for further explanation.

Value

List With

Posteriors: (1:N,1:L) of Posteriors corresponding to Data

NormalizationFactor: (1:N) denominator of Bayes theorem corresponding to Data

Author(s)

Alfred Ultsch, Michael Thrun

10 CDFMixtures

References

Thrun M.C., Ultsch, A.: Models of Income Distributions for Knowledge Discovery, European Conference on Data Analysis, DOI 10.13140/RG.2.1.4463.0244, Colchester 2015.

See Also

BayesDecisionBoundaries,AdaptGauss

CDFMixtures

cumulative distribution of mixture model

Description

returns the cdf (cumulative distribution function) of a mixture model of gaussian or log gaussians

Usage

```
CDFMixtures(Kernels, Means, SDs, Weights, IsLogDistribution)
```

Arguments

Kernels at these locations N(Means, Sdevs)*Weights is used for cdf calcuation, NOTE:

Kernels are usually (but not necessarily) sorted and unique

Means vector(1:L), Means of Gaussians, L == Number of Gaussians

SDs estimated Gaussian Kernels = standard deviations

Weights optional, relative number of points in Gaussians (prior probabilities): sum(Weights)

==1, default weight is 1/L

 ${\tt IsLogDistribution}$

Optional, if IsLogDistribution(i)==1, then mixture is lognormal default == 0*(1:L)

Value

List with

CDFGaussMixture

(1:N,1), cdf of Sum of SingleGaussians at Kernels

CDFSingleGaussian

(1:N,1:L),cdf of mixtures at Kernels

Author(s)

Rabea Griese

See Also

Chi2testMixtures

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Chi2testMixtures	Pearson's chi-squared goodness of fit test	

Description

Chi2testMixtures is goodness of fit test which establishes whether an observed distribution (data) differs from a Gauss Mixture Model (GMM). Returns a P value of a special case of a chi-square test and visualizes data versus a given GMM.

Usage

```
Chi2testMixtures(Data, Means, SDs, Weights,
IsLogDistribution, PlotIt, UpperLimit, VarName, NoRepetitionst)
```

Arguments

Data	vector of data points	(1:n)
------	-----------------------	-------

Means vector of Means of Gaussians (1:c)

SDs vector of standard deviations, estimated Gaussian Kernels (1:c)

Weights vector of relative number of points in Gaussians (prior probabilities) (1:c)

 ${\tt IsLogDistribution}$

Optional, if IsLogDistribution(i)==1, then mixture is lognormal, default vector

of zeros of length 1:L

PlotIt Optional, Default: FALSE, do a Plot of the compared cdfs and the KS-test dis-

tribution (Diff)

UpperLimit Optional. test only for Data <= UpperLimit, Default = max(Data) i.e all Data.

VarName If PlotIt=TRUE, the name of the inspected variable, default 'Data'

NoRepetitions Optional, scalar, default =1000, Number of Repetitions for monte carlo sam-

pling

Details

The null hypothesis is that the estimated data distribution does not differ significantly from the GMM. Let O_i be the observed features and E_i be the expected number E, than the test statistic is defined with the minimum chi-square estimate T=sum((O_i-E_i)^2/E_i)*1/m, where m the number of data points. The expected number Ei may be derived for each bin. If there is a significant difference between the O_i and the E_i, the Pvalue is small and the null hypothesis can be rejected.

Further details, see [Thrun & Ultsch, 2015].

Value

List with

Pvalue Pvalue of a suiting chi-square, Pvalue ==0 if Pvalue <0.001

BinCenters bin centers

ObsNrInBin No. of data in bin

ExpectedNrInBin

No. of data that should be in bin according to GMM

Chi 2Value the TestStatistic T i.e.: sum((ObsNrInBin(Ind)-ExpectedNrInBin(Ind))^2/ExpectedNrInBin(Ind))

with Ind = find(ExpectedNrInBin>=10) The value of Chi 2Value is compared to

a chi-squared distribution.

Note

The statistic assumption is that the test statistic follows a chi square distribution. The number of degrees of freedom is equal to the number of datapoints n-1-3*c

Author(s)

Rabea Griese, Michael Thrun

References

Hartung, J., Elpelt, B., and Kloesener, K.H.: Statistik, 8. Aufl. Verlag Oldenburg (1991).

Thrun, M. C., Ultsch, A.: Models of Income Distributions for Knowledge Discovery, European Conference on Data Analysis, DOI 10.13140/RG.2.1.4463.0244, pp. 28-29, Colchester 2015.

ClassifyByDecisionBoundaries

Classify Data according to decision Boundaries

Description

The Decision Boundaries calculated through Bayes Theorem.

Usage

ClassifyByDecisionBoundaries(Data,DecisionBoundaries,ClassLabels)

Arguments

Data vector of Data

DecisionBoundaries

decision boundaries, BayesDecisionBoundaries

ClassLabels Optional numbered class labels that are assigned to the classes. default (1:L), L

number of different components of gaussian mixture model

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Value

Cls(1:n,1:d) classiffication of Data, such that 1= first component of gaussian mixture model, 2= second component of gaussian mixture model and so on. For Every datapoint a number is returned.

Author(s)

Michael Thrun

References

Duda, R. O., Hart, P. E., & Stork, D. G. (2001). Pattern classification. 2nd. Edition. New York, p. 512ff

See Also

BayesDecisionBoundaries, Bayes4Mixtures

EMGauss

EM Algorithm for GMM

Description

Expectation-Maximization algorithm to calculate optimal Gaussian Mixture Model for given data in one Dimension.

Usage

EMGauss(Data, K, Means, SDs, Weights, MaxNumberofIterations, fast)

Arguments

Data vector of data points

K estimated amount of Gaussian Kernels

Means vector(1:L), Means of Gaussians, L == Number of Gaussians

SDs estimated Gaussian Kernels = standard deviations

Weights optional, relative number of points in Gaussians (prior probabilities): sum(Weights)

==1, default weight is 1/L

MaxNumberofIterations

Optional, Number of Iterations; default=10

fast Default: FALSE: Using mclust's EM see function densityMclust of that pack-

age, TRUE: Naive but faster EM implementation, which may be numerical un-

stable, because log(gauss) is not used

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Details

No adding or removing of Gaussian kernels. Number of Gaussian hast to be set by the length of the vector of Means, SDs and Weights. This EM is only for univariate data. For multivariate data see package mclust

Value

List with

Means means of GMM generated by EM algorithm

SDs standard deviations of GMM generated by EM algorithm

Weights prior probabilities of Gaussians

Author(s)

Onno Hansen-Goos, Michael Thrun, Florian Lerch

References

Bishop, Christopher M. Pattern recognition and machine learning. springer, 2006, p 435 ff

See Also

AdaptGauss

GMMplot_ggplot2

Plots the Gaussian Mixture Model (GMM) withing ggplot2

Description

PlotMixtures and PlotMixturesAndBoundaries for ggplot2

Usage

```
GMMplot_ggplot2(Data, Means, SDs, Weights,
BayesBoundaries, SingleGausses = TRUE, Hist = FALSE)
```

Arguments

Data vector (1:N) of data points

Means vector[1:L] of Means of Gaussians (of GMM),L == Number of Gaussians

SDs vector of standard deviations, estimated Gaussian Kernels, has to be the same

length as Means

Weights vector of relative number of points in Gaussians (prior probabilities), has to be

the same length as Means

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BayesBoundaries

Optional, x values for baye boundaries, if missing 'BayesDecisionBoundaries'

is called

SingleGausses Optional, SingleGausses=T than components of the mixture in blue will be

shown.

Hist Optional, geom_histogram overlayed

Value

```
ggplot2 object
```

Note

MT standardized code for CRAN and added dec boundaries and doku

Author(s)

```
Joern Loetsch, Michael Thrun (ctb)
```

See Also

PlotMixturesAndBoundaries, PlotMixtures, BayesDecisionBoundaries

Examples

```
data=c(rnorm(1000),rnorm(2000)+2,rnorm(1000)*2-1)
GMMplot_ggplot2(data,c(-1,0,2),c(2,1,1),c(0.25,0.25,0.5),SingleGausses=TRUE)
```

 $Information {\tt Criteria4GMM}$

Information Criteria For GMM

Description

Calculates the AIC and BIC criteria

Usage

```
InformationCriteria4GMM(Data, Means, SDs, Weights, IsLogDistribution)
```

Arguments

Data vector (1:N) of data points

Means vector[1:L] of Means of Gaussians (of GMM),L == Number of Gaussians

SDs vector of standard deviations, estimated Gaussian Kernels, has to be the same

length as Means

Weights vector of relative number of points in Gaussians (prior probabilities), has to be

the same length as Means

IsLogDistribution

Optional, ==1 if distribution(i) is a LogNormal, default vector of zeros of length

L, LogNormal Modes are at this point only experimental

Details

AIC = 2*k -2*LogLikelihood, k = nr. of model parameter = 3*Nr. of Gaussians One Gaussian: K=2 (Weight is then not an parameter!) SMALL SAMPLE CORRECTION: for n= nr of Data and n < 40*k, AIC is adjusted to AIC=AIC+ (2*k*(k+1))/(n-k-1)

BIC = k* log(n) - 2*LogLikelihood

Only for a Gaussian Mixture Model (GMM) verified, for the Log Gaussian, Gaussian, Log Gaussian (LGL) Model only experimental

Value

List with

K Number of gaussian mixturesAIC Akaike Informations criteriumBIC Bayes Information criterium

LogLikelihood of GMM, see LogLikelihood4Mixtures

PDFmixture probability density function of GMM, see Pdf4Mixtures

LogPDFdata log(PDFmixture)

Author(s)

Michael Thrun

References

Aubert, A. H., Thrun, M. C., Breuer, L., & Ultsch, A.: Knowledge discovery from data structure: hydrology versus biology controlled in-stream nitrate concentration, Scientific reports, Vol. (in revision), pp., 2016.

Aho, K., Derryberry, D., & Peterson, T.: Model selection for ecologists: the worldviews of AIC and BIC. Ecology, 95(3), pp. 631-636, 2014.

Intersect2Mixtures 17

Description

Finds the intersect of two gaussians or log gaussians

Usage

Intersect2Mixtures(Mean1,SD1,Weight1,Mean2,SD2,Weight2,IsLogDistribution,MinData,MaxData)

Arguments

Mean1 mean of 1.gaussian

SD1 standard deviations of 1.gaussian

Weight1 weight of 1. guassian
Mean2 mean of 2.gaussian

SD2 standard deviations of 2.gaussian

Weight 2 weight of 2. guassian

 ${\tt IsLogDistribution}$

Optional, ==1 if distribution(i) is a LogNormal, default vector of zeros of length

2

MinData Optional, Beginning of range, where the intersect is searched for, default min(Mean1,Mean2)

MaxData Optional, End of range, where the intersect is searched for, default max(Mean1,Mean2)

Value

CutX x value, where gaussian 1=gaussian2
CutY y value, where gaussian 1=gaussian2

Author(s)

Michael Thrun, Rabea Griese

See Also

BayesDecisionBoundaries

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KStestMixtures	Kolmogorov-Smirnov test

Description

Returns a P value and visualizes for Kolmogorov-Smirnov test of Data versus a given Gauss Mixture Model

Usage

```
KS test \verb|Mixtures| (Data, \verb|Means|, SDs|, \verb|Weights|, IsLogDistribution|, IslogDist
```

PlotIt, UpperLimit, NoRepetitions, Silent)

Arguments

Data vector of data points

Means vector of Means of Gaussians

SDs vector of standard deviations, estimated Gaussian Kernels

Weights vector of relative number of points in Gaussians (prior probabilities)

IsLogDistribution

Optional, if IsLogDistribution(i)==1, then mixture is lognormal, default vector

of zeros of length 1:L

PlotIt Optional, Default: FALSE, do a Plot of the compared cdfs and the KS-test dis-

tribution (Diff)

UpperLimit Optional. test only for Data <= UpperLimit, Default = max(Data) i.e all Data.

NoRepetitions Optional, default =1000, scalar, Number of Repetitions for monte carlo sam-

pling

Silent Optional, default=TRUE, If FALSE, shows progress of computation by points

(On windows systems a progress bar)

Details

The null hypothesis is that the estimated data distribution does not differ significantly from the GMM. If there is a significant difference, then the Pvalue is small and the null hypothesis is rejected.

Value

List with

Pvalue Pvalue of a suiting Kolmogorov-Smirnov test, Pvalue ==0 if Pvalue <0.001

DataKernels such that plot(DataKernels,DataCDF) gives the cdf(Data)

DataCDF such that plot(DataKernels,DataCDF) gives the cdf(Data)

 ${\tt CDFGaussMixture}$

No. of data that should be in bin according to GMM

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Author(s)

Michael Thrun, Alfred Ultsch

References

Smirnov, N., Table for Estimating the Goodness of Fit of Empirical Distributions. 1948, (2), 279-281.

LikelihoodRatio4Mixtures

Likelihood Ratio for Gaussian Mixtures

Description

Computes the likelihood ratio for two Gaussian Mixture Models.

Usage

LikelihoodRatio4Mixtures(Data, NullMixture, OneMixture, PlotIt, LowerLimit, UpperLimit)

Arguments

Data	Data points.
NullMixture	A Matrix: cbind(Means0,SDs0,Weights0) or cbind(Means0,SDs0,Weights0,IsLog0). The null model; usually with less Gaussians than the OneMixture
OneMixture	A Matrix: cbind(Means1,SDs1,Weights1) or cbind(Means1,SDs1,Weights1,IsLog1). The alternative model usually with more Gaussians than the OneMixture.
PlotIt	Optional: zero or one. o a Plot of the compared cdf's and the KS-test distribution (Diff)
LowerLimit	Optional: test only for Data >= LowerLimit, Default = min(Data) i.e all Data.
UpperLimit	Optional: test only for Data <= UpperLimit, Default = max(Data) i.e all Data.

Value

List with

Pvalue the error that we make, if we accept OneMixture as the better Model over the

NullMixture

NullLogLikelihood

log likelihood of GMM Null

OneLogLikelihood

log likelihood of GMM One

Author(s)

Alfred Ultsch, Michael Thrun, Catharina Lippmann

Examples

```
data2=c(rnorm(1000),rnorm(2000)+2,rnorm(1000)*2-1)
## Not run: Vals=AdaptGauss(data2,c(-1,0,2),c(2,1,1),c(0.25,0.25,0.5),0.3,-6,6)
NullMixture=cbind(Vals$Means,Vals$SDs,Vals$Weights)

## End(Not run)
## Not run: Vals2=AdaptGauss(data2,c(-1,0,2,3),c(2,1,1,1),c(0.25,0.25,0.25,0.25),0.3,-6,6)
OneMixture=cbind(Vals2$Means,Vals2$SDs,Vals2$Weights)

## End(Not run)
## Not run:
res=LikelihoodRatio4Mixtures(Data,NullMixture,OneMixture,T)
## End(Not run)
```

LKWFahrzeitSeehafen2010

Truck driving time seaport 2010

Description

Truck driving time to seaports measured in 2010.

Usage

```
data("LKWFahrzeitSeehafen2010")
```

Format

The format is: num [1:11441] 84.7 13.2 11.5 41.4 52.9 ...

References

Behnisch, M., Ultsch, A.: Knowledge Discovery in Spatial Planning Data - A Concept for Cluster Understanding, in: Helbich, M., Arsanjani, J. J., Leitner, M. (eds.): Computational Approaches for Urban Environments, in: Gatrell, J.D., Jensen, R.R.: Geotechnologies and the Environment Series, Vol, 13, Springer, Berlin, pp. 49-75, 2015.

Examples

```
data(LKWFahrzeitSeehafen2010)
## maybe str(LKWFahrzeitSeehafen2010) ; plot(LKWFahrzeitSeehafen2010) ...
```

LogLikelihood4Mixtures

LogLikelihood for Gaussian Mixture Models

Description

Computes the LogLikelihood for Gaussian Mixture Models.

Usage

LogLikelihood4Mixtures(Data, Means, SDs, Weights, IsLogDistribution)

Arguments

Data for empirical PDF. Has to be an Array of values. NaNs and NULLs will be

deleted

Means Optional: Means of gaussians of GMM.

SDs Optional: StandardDevations of gaussians of GMM. (Has to be the same length

as Means)

Weights Optional: Weights of gaussians of GMM. (Has to be the same length as Means)

 ${\tt IsLogDistribution}$

Optional, ==1 if distribution(i) is a LogNormal, default vector of zeros of length

1:L

Value

List with

LogLikelihood = = sum(log(PDFmixture)

 $\mathsf{LogPDF} \qquad \qquad \mathsf{=log}(PDFmixture)$

PDFmixture die Probability density function for each point

Author(s)

Alfred Ultsch, Catharina Lippmann

References

Pattern Recognition and Machine Learning, C.M. Bishop, 2006, isbn: ISBN-13: 978-0387-31073-2, p. 433 (9.14)

22 Pdf4Mixtures

|--|

Description

Calculate Gaussianthe probability density function for a Mixture Model

Usage

```
Pdf4Mixtures(Data, Means, SDs, Weights, IsLogDistribution, PlotIt)
```

Arguments

Data vector (1:N) of data points

Means vector[1:L] of Means of Gaussians (of GMM),L == Number of Gaussians

SDs vector of standard deviations, estimated Gaussian Kernels, has to be the same

length as Means

Weights vector of relative number of points in Gaussians (prior probabilities), has to be

the same length as Means

IsLogDistribution

Optional, ==1 if distribution(i) is a LogNormal, default vector of zeros of length

I:L

PlotIt Optional: =TRUE plot of pdf

Value

List with

PDF4modes matrix, where the columns are the gaussians

PDF matrix, where the columns are the gaussians weighted by Weights
PDFmixture linear superpositions of PDF - prior probabilities of Gaussians

Author(s)

Michael Thrun

See Also

PlotMixtures

Examples

```
 \begin{array}{l} {\tt data=c(rnorm(1000),rnorm(2000)+2,rnorm(1000)*2-1)} \\ {\tt Pdf4Mixtures(data,c(-1,0,2),c(2,1,1),c(0.25,0.25,0.5), \ PlotIt=TRUE)} \end{array}
```

PlotMixtures 23

Description

Plots Gaussian Mixture Model without Bayes decision boundaries, such that:

Black is the PDE of Data

Red is color of the GMM

Blue is the color of components of the mixture

Arguments

Data	vector (1:N) of data points	
Means	vector[1:L] of Means of Gaussians (of GMM),L == Number of Gaussians	
SDs	vector of standard deviations, estimated Gaussian Kernels, has to be the same length as Means	
Weights	vector of relative number of points in Gaussians (prior probabilities), has to be the same length as Means	
IsLogDistribution		
	Optional, ==1 if distribution(i) is a LogNormal, default vector of zeros of length 1:L	
Plotter	Optional, plotting package, either native or plotly	
SingleColor	Optional, Color for line plot of all the single gaussians, default magenta	
MixtureColor	Optional, Color of line lot for the mixture default red	
DataColor	Optional, Color of line plot for the data, default black	
SingleGausses	Optional, If TRUE, single gaussians are shown, default FALSE	
axes	Optional, Default: TRUE with axis, see argument axis of plot	
xlab	Optional, see plot	
ylab	Optional, see plot	
xlim	Optional, see plot	
ylim	Optional, see plot	
ParetoRad	Optional: Precalculated Pareto Radius to use	

Details

. . .

Example shows that overlapping variances of gaussians will result in inappropriate decision boundaries.

other plot arguments like $x \lim = c(1,10)$

Author(s)

Michael Thrun, Quirin Stier

See Also

PlotMixturesAndBoundaries

Examples

```
 \label{eq:data} $$ \data=c(rnorm(1000),rnorm(2000)+2,rnorm(1000)*2-1)$$ $$ PlotMixtures(data,c(-1,0,2),c(2,1,1),c(0.25,0.25,0.5),SingleColor='blue',SingleGausses=TRUE) $$ $$ \data=c(rnorm(1000),rnorm(2000)+2,rnorm(1000)*2-1)$$ $$ \data=c(rnorm(1000),rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,rnorm(2000)+2,r
```

PlotMixturesAndBoundaries

Shows GMM with Boundaries

Description

Plots Gaussian Mixture Model with Bayes decision boundaries, such that:

Black is the PDE of Data

Red is color of the GMM

Magenta are the Bayes boundaries

Usage

```
PlotMixturesAndBoundaries(Data, Means, SDs, Weights,

IsLogDistribution = rep(FALSE, length(Means)), Plotter="native",

SingleColor = "blue", MixtureColor = "red", DataColor = "black",

BoundaryColor = "magenta", xlab, ylab,

SingleGausses =TRUE, ...)
```

Arguments

Data vector (1:N) of data points

Means vector[1:L] of Means of Gaussians (of GMM),L == Number of Gaussians

SDs vector of standard deviations, estimated Gaussian Kernels, has to be the same

length as Means

Weights vector of relative number of points in Gaussians (prior probabilities), has to be

the same length as Means

IsLogDistribution

Optional, ==1 if distribution(i) is a LogNormal, default vector of zeros of length

1:L

Plotter Optional, plotting package, either native or plotly

QQplotGMM 25

SingleColor Optional, Color for line plot of all the single gaussians, default magenta

MixtureColor Optional, Color of line plot for the mixture, default red

DataColor Optional, Color of line plot for the data, default black

BoundaryColor Optional, Color of bayesian boundaries

xlab Optional, x label, see plot ylab Optional, y label, ee plot

SingleGausses Optional, SingleGausses=T than components of the mixture in blue will be

shown.

... Optional, see plot for plot properties and for SingleGausses PlotMixtures

Author(s)

Michael Thrun

See Also

BayesDecisionBoundaries,PlotMixtures

QQplotGMM Quantile Quantile Plot of Data

Description

Quantile Quantile plot of data against gaussian distribution mixture model with optional best-fit-line

Usage

```
QQplotGMM(Data, Means, SDs, Weights, IsLogDistribution, Line, PlotSymbol, xug, xog, LineWidth, PointWidth, ylab, main, ...)
```

Arguments

Data vector (1:N) of data points

Means vector[1:L] of Means of Gaussians (of GMM),L == Number of Gaussians

SDs vector of standard deviations, estimated Gaussian Kernels, has to be the same

length as Means

Weights vector of relative number of points in Gaussians (prior probabilities), has to be

the same length as Means

IsLogDistribution

Optional, ==1 if distribution(i) is a LogNormal, default Zeros of Length L

Line Optional, Default: TRUE=Regression Line is drawn

xug Optional, lower limit of the interval [xug, xog], in which a line will be interpo-

lated

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xog Optional, upper limit of the interval [xug, xog], in which a line will be interpo-

lated

PlotSymbol Optional, plot symbol. Default is 20.

LineWidth Optional, width of regression line, if Line==TRUE

PointWidth Optional, width of points

ylab Optional, see plot main Optional, see plot

... Note: xlab cannot be changed, other parameters see qqplot

Details

Only verified for a Gaussian Mixture Model, usage of IsLogDistribution for LogNormal Modes is experimental!

Value

List with

x The x coordinates of the points that were plotted

y The original data vector, i.e., the corresponding y coordinates

Author(s)

Michael Thrun

References

Michael, J. R. (1983). The stabilized probability plot. Biometrika, 70(1), 11-17.

See Also

qqplot

Examples

```
data=c(rnorm(1000),rnorm(2000)+2,rnorm(1000)*2-1)
QQplotGMM(data,c(-1,0,2),c(2,1,1),c(0.25,0.25,0.5))
```

RandomLogGMM 27

RandomLogGMM	Random Number Generator for Log or Gaussian Mixture Model

Description

Function finds the intersections of Gaussians or LogNormals

Usage

RandomLogGMM(Means,SDs,Weights,IsLogDistribution,TotalNoPoints)

Arguments

Means vector[1:L] of Means of Gaussians (of GMM)

SDs vector of standard deviations, estimated Gaussian Kernels, has to be the same

length as Means

Weights vector of relative number of points in Gaussians (prior probabilities), has to be

the same length as Means

 ${\tt IsLogDistribution}$

Optional, ==1 if distribution(i) is a LogNormal, default vector of Zeros of Length

L

TotalNoPoints Optional, number of point for log or GMM generated

Value

Returns vector of [1:TotalNoPoints] of genrated points for log oder gaussian mixture model

Author(s)

Alfred Ultsch, Michael Thrun, Rabea Griese

See Also

QQplotGMM,Chi2testMixtures

28 Symlognpdf

Symlognpdf	computes a special case of log normal distribution density

Description

Symlognpdf is an internal function for AdaptLGL.

Usage

```
Symlognpdf(Data, Mean, SD)
```

Arguments

Data vector of data points used for sampling

Mean of log Gaussian

SD Standard deviation of log Gaussian

Value

M>0 Log normal distribution density

M<0 Log normal distribution density mirrored at y axis

Note

not for external usage.

See Also

AdaptLGL

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