Package: DistributionOptimization (via r-universe)

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Description Fits Gaussian Mixtures by applying evolution. As fitness function a mixture of the chi square test for distributions and a novel measure for approximating the common area under curves between multiple Gaussians is used. The package presents an alternative to the commonly used Likelihood Maximization as is used in Expectation Maximization. The algorithm and applications of this package are published under: Lerch, F., Ultsch, A., Lotsch, J. (2020) <doi:10.1038 s41598-020-57432-w="">. The evolution is based on the 'GA' package: Scrucca, L. (2013) <doi:10.18637 jss.v053.i04=""> while the Gaussian Mixture Logic stems from 'AdaptGauss': Ultsch, A, et al. (2015) <doi:10.3390 ijms161025897="">.</doi:10.3390></doi:10.18637></doi:10.1038>
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Distribution Optimization

Description

Distribution Optimization fits gaussian mixture models on to one dimensional samples by minimizing the Chi Squared Error by evolutional optimization. It is an alternative to likelihood maximizers like expection maximization. Through the included "Overlapping" Methods, single gaussians can be forced to be separated, achieving various significant models to choose from. The evolutionary part is done through the "GA" Package. The Gaussian Mixture Logic is based on the "AdaptGauss" Package.

Author(s)

Florian Lerch, Jorn Lotsch, Alfred Ultsch

References

Luca Scrucca (2013). GA: A Package for Genetic Algorithms in R. Journal of Statistical Software, 53(4), 1-37. URL http://www.jstatsoft.org/v53/i04/

BinProb4Mixtures

Bin Probabilities

Description

Calculates the probability of bins/intervals within the dataspace defined by given breaks between them.

Usage

```
BinProb4Mixtures(Means, SDs, Weights, Breaks, IsLogDistribution = rep(F,
  length(Means)), LimitsAreFinite = T)
```

Arguments

Means of the GMM Components

SDs Standard Deviations of the GMM Components

Weights Weights of the GMM Components

Breaks Defining c-1 or c+1 bins (depending on LimitsAreFinite)

IsLogDistribution

If True, the GMM is interpreted as a logarithmic

LimitsAreFinite

If True, there are c+1 Bins, where the first and last bin are of inifinite size

Value

Probabalities of either c-1 or c+1 bins/intervals (depending on LimitsAreFinite)

Author(s)

Florian Lerch

Examples

```
Data = c(rnorm(50,1,2), rnorm(50,3,4))
NoBins = 20
breaks = seq(min(Data), max(Data), length.out=length(NoBins)+1)
BinProb4Mixtures(c(1,3), c(2,4), c(0.5,0.5), breaks)
```

DistributionOptimization

Distribution Fitting

Description

Fits a Gaussian Mixture Model onto a Dataset by minimizing a fitting error through evolutionary optimization. Every individual encodes one GMM. Details over the evolutionary process itself can be taken from the 'GA' package. ga

Usage

```
DistributionOptimization(Data, Modes, Monitor = 1,
    SelectionMethod = "UnbiasedTournament",
    MutationMethod = "Uniform+Focused",
    CrossoverMethod = "WholeArithmetic", PopulationSize = Modes * 3 * 25,
    MutationRate = 0.7, Elitism = 0.05, CrossoverRate = 0.2,
    Iter = Modes * 3 * 200, OverlapTolerance = NULL,
    IsLogDistribution = rep(F, Modes), ErrorMethod = "chisquare",
    NoBins = NULL, Seed = NULL, ConcurrentInit = F, ParetoRad = NULL)
```

Arguments

Data to be modelled

Modes Number of expected Modes

Monitor 0:no monitoring, 1: status messages, 2: status messages and plots, 3: status

messages, plots and calculated error-measures

SelectionMethod

1: LinearRank selection 4: UnbiasedTournament 5: FitnessProportional selec-

tion

MutationMethod 1: UniformRandom mutation 2: NonuniformRandom mutation 4: Focused mu-

tation, alternative random mutation around solution 5: GaussMutationCust 6: TwoPhaseMutation - mutation is uniform random during the first half of itera-

tions, and than focuses around current solution

CrossoverMethod

1: single point crossover 2: whole arithmetic crossover 3: local arithmetic crossover 4: blend crossover 5: GaussCrossover - exchange complete gaussian components 6: MultiPointCrossover - Random amount of information between

mixtures get exchanged

PopulationSize Size of the population

MutationRate amount (0..1) of population that gets mutated

Elitism amount of best individuals that will survive generation unchanged

CrossoverRate amount of individuals that will be used for crossover

Iter number of iterations of this algorithm

OverlapTolerance

ratio between Chi-Square and OverlapError (only if FitnessMethod = 4 (Chi2ValueWithOverlap))

 ${\tt IsLogDistribution}$

which gauss components should be considered as log gaussian

ErrorMethod "pde": fitting is measured by pareto density estimation. "chisquare": fitting is

measured by Chi-Square test

NoBins Number of Bins that will be used for evaluating fitting

Seed Random Seed for reproducible results

ConcurrentInit If true, before initialization a number of short optimizations are done to find a

good starting point for evolution

ParetoRad Pareto Radius for Pareto Density Estimation and its plots

Value

The GA object containing the evolutionary training and a description of the final GMM consisting of means, sdevs and weights.

Author(s)

Florian Lerch

Jorn Lotsch

Alfred Ultsch

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Examples

```
## Not run:
DistributionOptimization(c(rnorm(200),rnorm(200,3), 2))
## End(Not run)
```

MixedDistributionError

MixedDistributionError

Description

Calculates a fitting error as well as the overlapping measure for the mixtures. Combines them with ratio rho in favor of Overlapping.

Usage

```
MixedDistributionError(Means, SDs, Weights, Data, rho = 0.5,
  breaks = NULL, Kernels = NULL, ErrorMethod = "chisquare")
```

Arguments

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SDs Standard Deviations of the GMM Components

Weights Weights of the GMM Components

Data Empirical Data based on which the GMM is build

rho Ratio of OverlappingError vs Fitting Error breaks vector containing the breaks between bins Kernels positions at which density is to be compared

ErrorMethod "pdeerror": fitting error is measured through Pareto Density Estimation. "chisquare":

fitting error is measured through the Chi Square fitting error.

Value

Mixed Error

Author(s)

Florian Lerch

Examples

```
Data = c(rnorm(50,1,2), rnorm(50,3,4))
MixedDistributionError(c(1,3), c(2,4), c(0.5,0.5), Data = Data)
```

OverlapErrorByDensity OverlapErrorByDensity

Description

Similarity in GMM by Density

Usage

```
OverlapErrorByDensity(Means, SDs, Weights, Data = NULL, Kernels = NULL)
```

Arguments

Means of the GMM Components

SDs Standard Deviations of the GMM Components

Weights Weights of the GMM Components

Data Dataset that the GMM should be compared with

Kernels if length(Kernels) = 1: amount of kernels if length(Kernels) > 1: kernels in

dataspace at which the GMM Components will be compared with each other

Details

Calculates the similarity (overlap) between multiple modes in Gaussian Mixture Models. Kernels at equally distanced positions are used, if not explicitly given.

Value

List: OverlapError Error for estimating the maximal Overlap of AUC of PDFs of each pair of GMM Components Kernels Kernels that were used for comparing the GMM Components

Author(s)

Florian Lerch

Examples

```
\label{eq:decomposition} \begin{array}{lll} \text{Data} = \text{c(rnorm(50,1,2), rnorm(50,3,4))} \\ \text{V<-OverlapErrorByDensity(c(1,3), c(2,4), c(0.5,0.5), Data} = \text{Data)} \\ \text{AdaptGauss::PlotMixtures(Data, c(1,3), c(2,4), SingleGausses} = \text{TRUE)} \\ \text{print(V$OverlapError)} \end{array}
```

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