## Package: LogConcDEAD (via r-universe)

September 12, 2024

Type Package

Title Log-Concave Density Estimation in Arbitrary Dimensions

Version 1.6-10

Date 2024-09-10

Depends R (>= 3.0)

Imports MASS, mclust, mvtnorm

**Suggests** rgl, tkrplot **Enhances** logcondens

**Description** Software for computing a log-concave (maximum likelihood) estimator for independent and identically distributed data in any number of dimensions. For a detailed description of the method see Cule, Samworth and Stewart (2010, Journal of Royal Statistical Society Series B, <doi:10.1111/j.1467-9868.2010.00753.x>).

**License** GPL (>= 2) **NeedsCompilation** yes

Author Madeleine Cule [aut], Robert Gramacy [aut], Richard Samworth [aut], Yining Chen [aut, cre], Lutz Duembgen [ctb] (helped improve the numerical stability), Vikneswaran Gopal [ctb] (proposed the Metropolis-Hastings scheme for draw samples from a log-concave distribution), George Casella [ctb] (proposed the Metropolis-Hastings scheme for draw samples from a log-concave distribution), C. Bradford Barber [cph] (author of the Qhull library), The Geometry Center [cph], Kai Habel [cph] (author of the function that imports convex hull computation from Qhull to R), Raoul Grasman [cph] (author of the function that imports convex hull computation from Qhull to R), Alexei Kuntsevich [cph] (author of the C function for Shor's r algorithm), Franz Kappel [cph] (author of the C function for Shor's r algorithm)

Maintainer Yining Chen < y.chen101@lse.ac.uk>

**Date/Publication** 2024-09-11 22:53:04 UTC **Repository** https://ychen101.r-universe.dev

RemoteUrl https://github.com/cran/LogConcDEAD

RemoteRef HEAD

**RemoteSha** bbd31770f1c83c0806e084b3427fa0a35fa31bdb

## **Contents**

LogCo	oncDEAD-package	Com data		_		,			um	li	kei	lih	00	d)	e	sti	im	ate	or	fe	or	i.	i.d	
Index																								28
	rslcd		 •	 •	 •	 •	 •	•	•		•	•	•	•	•	•	•		•	٠	٠	•	•	26
	rlcd																							
	print.LogConcDEAl																							
	plot.LogConcDEAD																							22
	mlelcd																							18
	interpmargled																							
	interpled																							
	hatA interactive2D																							
	getweights																							
	getinfoled																							
	EMmixled																							
	dslcd																							
	dmarglcd																							7
	dlcd																							5
	cov.LogConcDEAD	_																						4
	LogConcDEAD-pac	kage					 																	2

## Description

This package contains a function to compute the maximum likelihood estimator of a log-concave density in any number of dimensions using Shor's r-algorithm.

Functions to plot (for 1- and 2-d data), evaluate and draw samples from the maximum likelihood estimator are provided.

#### **Details**

This package contains a selection of functions for maximum likelihood estimation under the constraint of log-concavity.

mlelcd computes the maximum likelihood estimator (specified via its value at data points). Output is a list of class "LogConcDEAD" which is used as input to various auxiliary functions.

hatA calculates the difference between the sample covariance and the fitted covariance.

dlcd evaluates the estimated density at a particular point.

dslcd evaluates the smoothed version of estimated density at a particular point.

rlcd draws samples from the estimated density.

rslcd draws samples from the smoothed version of estimated density.

interplcd interpolates the estimated density on a grid for plotting purposes.

dmarglcd evaluates the estimated marginal density by integrating the estimated density over an appropriate subspace.

interpmarglcd evaluates a marginal density estimate at equally spaced points along the axis for plotting purposes. This is done by integrating the estimated density over an appropriate subspace.

plot.LogConcDEAD produces plots of the maximum likelihood estimator, optionally using the **rgl** package.

print and summary methods are also available.

#### Note

The authors gratefully acknowledge the assistance of Lutz Duembgen at the University of Bern for his insight into the objective function in mlelcd.

For one dimensional data, the active set algorithm in logcondens is much faster.

## Author(s)

Yining Chen (maintainer) < y.chen101@lse.ac.uk>

Madeleine Cule

Robert Gramacy

Richard Samworth

#### References

Barber, C.B., Dobkin, D.P., and Huhdanpaa, H.T. (1996) *The Quickhull algorithm for convex hulls* ACM Trans. on Mathematical Software, 22(4) p.469-483 http://www.qhull.org

Chen, Y. and Samworth, R. J. (2013) *Smoothed log-concave maximum likelihood estimation with applications* Statist. Sinica, 23, 1373-1398. https://arxiv.org/abs/1102.1191v4

Cule, M. L. and Duembgen, L. (2008) *On an auxiliary function for log-density estimation*, University of Bern technical report. https://arxiv.org/abs/0807.4719

Cule, M. L., Samworth, R. J., and Stewart, M. I. (2010) *Maximum likelihood estimation of a multi-dimensional log-concave density* J. Roy. Statist. Soc., Ser. B. (with discussion), 72, 545-600.

Gopal, V. and Casella, G. (2010) Discussion of Maximum likelihood estimation of a log-concave density by Cule, Samworth and Stewart J. Roy. Statist. Soc., Ser. B., 72, 580-582.

Grundmann, A. and Moeller, M. (1978) *Invariant Integration Formulas for the N-Simplex by Combinatorial Methods* SIAM Journal on Numerical Analysis, Volume 15, Number 2, 282-290.

Kappel, F. and Kuntsevich, A. V. (2000) *An implementation of Shor's r-algorithm* Computational Optimization and Applications, Volume 15, Issue 2, 193-205.

Shor, N. Z. (1985) Minimization methods for nondifferentiable functions Springer-Verlag

4 cov.LogConcDEAD

#### See Also

```
logcondens, rgl
```

#### **Examples**

```
## Some simple normal data, and a few plots
x <- matrix(rnorm(200),ncol=2)</pre>
lcd \leftarrow mlelcd(x)
g <- interplcd(lcd)</pre>
oldpar <- par(mfrow = c(1,1))
par(mfrow=c(2,2), ask=TRUE)
plot(lcd, g=g, type="c")
plot(lcd, g=g, type="c", uselog=TRUE)
plot(lcd, g=g, type="i")
plot(lcd, g=g, type="i", uselog=TRUE)
par(oldpar)
## Some plots of marginal estimates
g.marg1 <- interpmarglcd(lcd, marg=1)</pre>
g.marg2 <- interpmarglcd(lcd, marg=2)</pre>
plot(lcd, marg=1, g.marg=g.marg1)
plot(lcd, marg=2, g.marg=g.marg2)
## generate some points from the fitted density
generated <- rlcd(100, lcd)</pre>
genmean <- colMeans(generated)</pre>
## evaluate the fitted density
mypoint <-c(0, 0)
dlcd(mypoint, lcd, uselog=FALSE)
mypoint <- c(10, 0)
dlcd(mypoint, lcd, uselog=FALSE)
## evaluate the marginal density
dmarglcd(0, lcd, marg=1)
dmarglcd(1, lcd, marg=2)
```

cov.LogConcDEAD

Compute the covariance matrix of a log-concave maximum likelihood estimator

## Description

This function computes the covariance matrix of a log-concave maximum likelihood estimator.

#### Usage

```
cov.LogConcDEAD(1cd)
```

dlcd 5

## **Arguments**

lcd

Object of class "LogConcDEAD" (typically output from mlelcd)

#### Details

This function evaluates the covariance matrix of a given log-concave maximum likelihood estimator using the second order partial derivatives of the auxiliary function studied in *Cule*, *M. L. and Duembgen*, *L.* (2008).

For examples, see mlelcd.

#### Value

A matrix equals the covariance matrix of the log-concave maximum likelihood density estimator.

#### Author(s)

Yining Chen

Madeleine Cule

Robert Gramacy

Richard Samworth

#### References

Cule, M. L. and Duembgen, L. (2008) On an auxiliary function for log-density estimation, University of Bern technical report. https://arxiv.org/abs/0807.4719

#### See Also

hatA

dlcd

Evaluation of a log-concave maximum likelihood estimator at a point

## Description

This function evaluates the density function of a log-concave maximum likelihood estimator at a point or points.

#### Usage

```
dlcd(x,lcd, uselog=FALSE, eps=10^-10)
```

6 dlcd

#### **Arguments**

х	Point (or matrix of points) at which the maximum likelihood estimator should be evaluated
lcd	Object of class "LogConcDEAD" (typically output from mlelcd)
uselog	Scalar logical: should the estimator should be calculated on the log scale?
eps	Tolerance for numerical stability

#### **Details**

A log-concave maximum likelihood estimate  $\hat{f}_n$  is satisfies  $\log \hat{f}_n = \bar{h}_y$  for some  $y \in \mathbb{R}^n$ , where

$$\bar{h}_y(x) = \inf\{h(x) : h \text{ concave }, h(x_i) \ge y_i \text{ for } i = 1, \dots, n\}.$$

Functions of this form may equivalently be specified by dividing  $C_n$ , the convex hull of the data into simplices  $C_j$  for  $j \in J$  (triangles in 2d, tetrahedra in 3d etc.), and setting

$$f(x) = \exp\{b_i^T x - \beta_j\}$$

for  $x \in C_j$ , and f(x) = 0 for  $x \notin C_n$ . The estimated density is zero outside the convex hull of the data

The estimate may therefore be evaluated by finding the appropriate simplex  $C_j$ , then evaluating  $\exp\{b_j^T x - \beta_j\}$  (if  $x \notin C_n$ , set f(x) = 0).

For examples, see mlelcd.

## Value

A vector of maximum likelihood estimate (or log maximum likelihood estimate) values, as evaluated at the points x.

#### Author(s)

Madeleine Cule

Robert Gramacy

Richard Samworth

#### See Also

mlelcd

dmargled 7

dmarglcd	Evaluate the marginal of multivariate log-concave maximum likeli- hood estimators at a point

## Description

Integrates the log-concave maximum likelihood estimator of multivariate data to evaluate the marginal density at a point.

## Usage

```
dmarglcd(x=0, lcd, marg=1)
```

## Arguments

Χ	Point (or vector of points) at which the marginal density is to be evaluated
lcd	Object of class "LogConcDEAD" (typically output from mlelcd)
marg	Which margin is required?

## **Details**

Given a multivariate log-concave maximum likelihood estimator in the form of an object of class "LogConcDEAD", a margin marg, and a real-valued point x, this function evaluates the estimated marginal density  $\hat{f}_{n,\text{marg}}(x)$ , as obtained by integrating over all the other dimensions.

For examples, see mlelcd.

## Value

A vector containing the values of the marginal density  $\hat{f}_{n, \text{marg}}$  at the points x.

## Author(s)

Madeleine Cule

Robert Gramacy

Richard Samworth

## See Also

mlelcd

8 dslcd

dslcd	Evaluation of a smoothed log-concave maximum likelihood estimator
	at given points

#### **Description**

This function evaluates the density function of a smoothed log-concave maximum likelihood estimator at a point or points.

#### Usage

```
dslcd(x, lcd, A=hatA(lcd))
```

#### **Arguments**

X	Point (or matrix of points) at which the smoothed log-concave maximum likelihood estimator should be evaluated
lcd	Object of class "LogConcDEAD" (typically output from mlelcd)
A	A positive definite matrix that determines the degree of smoothing, typically taken as the output of hatA(lcd)

#### **Details**

The smoothed log-concave maximum likelihood estimator is a fully automatic nonparametric density estimator, obtained as a canonical smoothing of the log-concave maximum likelihood estimator. More precisely, it equals the convolution  $\hat{f}*\phi_{d,\hat{A}}$ , where  $\phi_{d,\hat{A}}$  is the density function of d-dimensional multivariate normal with covariance matrix  $\hat{A}$ . Typically,  $\hat{A}$  is taken as the difference between the sample covariance and the covariance of fitted log-concave maximum likelihood density. Therefore, this estimator matches both the empirical mean and empirical covariance.

The estimate is evaluated numerically either by Gaussian quadrature in two dimensions, or in higher dimensions, via a combinatorial method proposed by *Grundmann and Moeller* (1978). Details of the computational aspects can be found in *Chen and Samworth* (2011). In one dimension, explicit expression can be derived. See logcondens for more information.

For examples, see mlelcd

#### Value

A vector of smoothed log-concave maximum likelihood estimate values, as evaluated at the points x.

#### Author(s)

Yining Chen

Madeleine Cule

Robert Gramacy

Richard Samworth

EMmixlcd 9

#### References

Chen, Y. and Samworth, R. J. (2013) *Smoothed log-concave maximum likelihood estimation with applications* Statist. Sinica, 23, 1373-1398. https://arxiv.org/abs/1102.1191v4

Grundmann, A. and Moeller, M. (1978) *Invariant Integration Formulas for the N-Simplex by Combinatorial Methods* SIAM Journal on Numerical Analysis, Volume 15, Number 2, 282-290.

#### See Also

dlcd, hatA, mlelcd

EMmixlcd	Estimate the mixture proportions and component densities using EM algorithm

## Description

Uses EM algorithm to estimate the mixture proportions and the component densities. The output is an object of class "lcdmix" which contains mixture proportions at each observation and all the information of the estimated component densities.

## Usage

## Arguments

X	Data in $\mathbb{R}^d$ , in the form of an $n \times d$ numeric matrix
k	The number of components, equals 2 by default
У	An $n \times k$ numeric matrix giving the starting values for the EM algorithm. If none given, a hierarchical Gaussian clustering model is used. To reduce the computational burden while allowing sufficient flexibility for the EM algorithm, it is recommended to leave this argument unspecified.
props	Vector of length $k$ containing the starting value of proportions. If none given, a hierarchical Gaussian clustering model is used. To reduce the computational burden while allowing sufficient flexibility for the EM algorithm, it is recommended to leave this argument unspecified.
epsratio	EM algorithm will terminate if the increase in the proportion of the likelihood is less than this specified ratio. Default value is $10^{-6}$ .
max.iter	The maximum number of iterations for the EM algorithm
epstheta	epstheta/n is the thresold of the weight below which data point is discarded from the cluster. This quantity is introduced to increase the computational efficiency and stability.
verbose	<ul> <li>-1: (default) prints nothing</li> <li>0: prints warning messages</li> </ul>
	• $> 0$ : prints summary information every $n$ iterations

10 EMmixled

#### **Details**

An introduction to the Em algorithm can be found in *McLachlan and Krishnan* (1997). Briefly, given the current estimates of the mixture proportions and component densities, we first update the estimates of the mixture proportions. We then update the estimates of the component densities by using mlelcd. In fact, the incorporation of the weights in the maximization process in mlelcd presents no additional complication.

In our case, because of the computational intensity of the method, we first cluster the points according to ta hierarchical Gaussian clustering model and then iterate the EM algorithm until the increase in the proportion of the likelihood is less than a pre-specified quantity at each step.

More technical details can be found in Cule, Samworth and Stewart(2010)

#### Value

An object of class "lcdmix", with the following components:

x Data copied from input (may be reordered)

logf An  $n \times k$  maxtrix of the log of the maximum likelihood estimate, evaluated at

the observation points for each component.

props Vector containing the estimated proportions of components

niter Number of iterations of the EM algorithm lcdloglik The log-likelihood after the final iteration

#### Author(s)

Yining Chen

Madeleine Cule

Robert B. Gramacy

Richard Samworth

#### References

Cule, M. L., Samworth, R. J., and Stewart, M. I. (2010) *Maximum likelihood estimation of a log-concave density*, Journal of the Royal Statistical Society, Series B, 72(5) p.545-607.

McLachlan, G. J. and Krishnan, T. (1997) The EM Algorithm and Extensions, New York: Wiley.

## See Also

```
mclust, logcondens, plot.LogConcDEAD, mlelcd, dlcd
```

#### **Examples**

```
##Simple bivariate normal data
  set.seed( 1 )
  n = 15
  d = 2
  props=c( 0.6, 0.4 )
  shift=2
```

getinfolcd 11

```
x <- matrix( rnorm( n*d ), ncol = d )
shiftvec <- ifelse( runif( n ) > props[ 1 ], 0, shift )
x[,1] <- x[,1] + shiftvec
EMmixlcd( x, k = 2, max.iter = 2)</pre>
```

getinfolcd

Construct an object of class LogConcDEAD

#### **Description**

A function to construct an object of class LogConcDEAD from a dataset (given as a matrix) and the value of the log maximum likelihood estimator at datapoints.

#### Usage

```
getinfolcd(x, y, w = rep(1/length(y), length(y)), chtol = 10^-6, MinSigma = NA, NumberOfEvaluations = NA)
```

#### **Arguments**

Data in  $R^d$ , in the form of an  $n \times d$  numeric matrix

y Value of log of maximum likelihood estimator at data points

We Vector of weights  $w_i$  such that the computed estimator maximizes

$$\sum_{i=1}^{n} w_i \log f(x_i)$$

subject to the restriction that f is log-concave. The default is  $\frac{1}{n}$  for all i, which corresponds to i.i.d. observations.

chtol Tolerance for computation of convex hull. Altering this is not recommended.

MinSigma Real-valued scalar giving minimum value of the objective function

NumberOfEvaluations

Vector containing the number of steps, number of function evaluations, and number of subgradient evaluations. If the **SolvOpt** algorithm fails, the first component will be an error code (<0)

#### **Details**

This function is used in mlelcd

12 getinfoled

#### Value

An object of class "LogConcDEAD", with the following components:

x Data copied from input (may be reordered)

w weights copied from input (may be reordered)

logMLE vector of the log of the maximum likelihood estimate, evaluated at the obser-

vation points

NumberOfEvaluations

Vector containing the number of steps, number of function evaluations, and number of subgradient evaluations. If the **SolvOpt** algorithm fails, the first com-

ponent will be an error code (< 0).

MinSigma Real-valued scalar giving minimum value of the objective function

b matrix containing row by row the values of  $b_j$ 's corresponding to each triangu-

lation; see also mlelcd

beta vector containing the values of  $\beta_i$ 's corresponding to each triangulation; see

also mlelcd

triang matrix containing final triangulation of the convex hull of the data

verts matrix containing details of triangulation for use in dlcd

vertsoffset matrix containing details of triangulation for use in dlcd

chull Vector containing vertices of faces of the convex hull of the data

outnorm matrix where each row is an outward pointing normal vectors for the faces of

the convex hull of the data. The number of vectors depends on the number of

faces of the convex hull.

outoffset matrix where each row is a point on a face of the convex hull of the data. The

number of vectors depends on the number of faces of the convex hull.

#### Author(s)

Madeleine Cule

Robert B. Gramacy

Richard Samworth

Yining Chen

#### See Also

mlelcd

getweights 13

getweights

Find appropriate weights for likelihood calculations

## **Description**

This function takes takes a matrix of (possibly binned) data and returns a matrix containing the distinct observations, and a vector of weights w as described below.

#### Usage

```
getweights(x)
```

#### **Arguments**

Х

a data matrix

#### **Details**

Given an  $n \times d$  matrix x of points in  $R^d$ , this function removes duplicated observations, and counts the number of times each observation occurs. This is used to compute a vector w such that

$$w_i = \frac{\# \text{ of times value } i \text{ is observed}}{\# \text{ of observations}}.$$

This function is called by mlelcd in order to compute the maximum likelihood estimator when the observed data values are not distinct. In this case, the log likelihood function is of the form

$$\sum_{j=1}^{m} w_j \log f(X_j),$$

where the sum is over distinct observations.

## Value

xout A matrix containing the distinct rows of the input matrix x

w A real-valued vector of weights as described above

## Author(s)

Madeleine Cule

Robert Gramacy

Richard Samworth

#### See Also

mlelcd

14 hatA

#### **Examples**

```
## simple normal example

x <- matrix(rnorm(200),ncol=2)
tmp <- getweights(x)
lcd <- mlelcd(tmp$x,tmp$w)
plot(lcd,type="ic")</pre>
```

hatA

Compute the smoothing matrix of the smoothed log-concave maximum likelihood estimator

## Description

This function computes the matrix  $\hat{A}$  of the smoothed log-concave maximum likelihood estimator

## Usage

hatA(lcd)

## **Arguments**

1cd

Object of class "LogConcDEAD" (typically output from mlelcd)

## **Details**

This function evaluates the the matrix  $\hat{A}$  of the smoothed log-concave maximum likelihood estimator, which is positive definite, and equals the difference between the sample covariance matrix and the covariance matrix of the fitted log-concave maximum likelihood density estimator.

For examples, see mlelcd

#### Value

A matrix equals  $\hat{A}$  of the smoothed log-concave maximum likelihood estimator

#### Note

Details of the computational aspects can be found in Chen and Samworth (2011).

## Author(s)

Yining Chen

Madeleine Cule

Robert Gramacy

Richard Samworth

interactive2D 15

#### References

Chen, Y. and Samworth, R. J. (2013) *Smoothed log-concave maximum likelihood estimation with applications* Statist. Sinica, 23, 1373-1398. https://arxiv.org/abs/1102.1191v4

#### See Also

cov.LogConcDEAD

interactive2D

A GUI for classification in two dimensions using smoothed log-concave

## **Description**

Uses tkrplot to create a GUI for two-class classification in two dimensions using the smoothed log-concave maximum likelihood estimates

## Usage

interactive2D(data, cl)

#### **Arguments**

data Data in  $R^2$ , in the form of an  $n \times 2$  numeric matrix

cl factor of true classifications of the data set

#### **Details**

This function uses tkrplot to create a GUI for two-class classification in two dimensions using the smoothed log-concave maximum likelihood estimates. The construction of the classifier is standard, and can be found in *Chen and Samworth (2013)*. The slider controls the risk ratio of two classes (equals one by default), which provides a way of demonstrating how the decision boundaries change as the ratio varies. Observations from different classes are plotted in red and green respectively.

#### Value

A GUI with a slider

## Author(s)

Yining Chen

Madeleine Cule

Robert B. Gramacy

Richard Samworth

16 interpled

#### References

Chen, Y. and Samworth, R. J. (2013) *Smoothed log-concave maximum likelihood estimation with applications* Statist. Sinica, 23, 1373-1398. https://arxiv.org/abs/1102.1191v4

Cule, M. L., Samworth, R. J., and Stewart, M. I. (2010) *Maximum likelihood estimation of a log-concave density*, Journal of the Royal Statistical Society, Series B, 72(5) p.545-607.

#### See Also

dslcd,mlelcd

## **Examples**

```
## Simple bivariate normal data
## only works interactively, not run as a test example here
if(interactive()){
    set.seed( 1 )
    n = 15
    d = 2
    props=c( 0.6, 0.4 )
    x <- matrix( rnorm( n*d ), ncol = d )
    shiftvec <- ifelse( runif( n ) > props[ 1 ], 0, 1)
    x[,1] <- x[,1] + shiftvec
    interactive2D( x, shiftvec )
}</pre>
```

interplcd

Evaluate the log-concave maximum likelihood estimator of 2-d data on a grid for plotting

## **Description**

Evaluates the logarithm of the log-concave maximum likelihood estimator on a grid for 2-d data, for use in plot.LogConcDEAD.

#### Usage

```
interplcd(lcd, gridlen=100 )
```

#### **Arguments**

1cd Object of class "LogConcDEAD" (typically output from mlelcd) gridlen A scalar indicating the size of the grid

#### **Details**

Interpolates the MLE over a grid.

The output is of a form readily usable by plot.LogConcDEAD, image, contour, etc, as illustrated in the examples below.

For examples, please see mlelcd.

interpmargled 17

#### Value

Χ	Vector of x-values of the grid
У	Vector of y-values of the grid
z	A matrix of the values of the log of the maximum likelihood estimator at points
	on the grid

## Author(s)

Madeleine Cule Robert Gramacy Richard Samworth

#### See Also

mlelcd

interpmarglcd	Finds marginals of multivariate logconcave maximum likelihood esti-
	mators by integrating

## **Description**

Integrates the maximum likelihood estimator of multivariate data over an appropriate subspace to produce axis-aligned marginals for use in plot.LogConcDEAD.

## Usage

```
interpmarglcd(lcd, marg=1, gridlen=100)
```

## Arguments

lcd Output from mlelcd (of class "LogConcDEAD")

marg An (integer) scalar indicating which margin is required gridlen An (integer) scalar indicating the size of the grid

## **Details**

Given a multivariate log-concave maximum likelihood estimator in the form of an object of class "LogConcDEAD" and a margin marg, this function will compute the marginal density estimate  $\hat{f}_{n,\text{marg}}$ . The estimate is evaluated at gridlen equally spaced points in the range where the density estimate is nonzero. These points are given in the vector xo.

 $f_{n,\text{marg}}$  is evaluated by integrating the log-concave maximum likelihood estimator  $\hat{f}_n$  over the other components. The marginal density is zero outside the range of xo.

For examples, see mlelcd.

#### Value

xo Vector of values at which the marginal density is estimate is computed.

marg Vector of values of the integrated maximum likelihood estimator at the locations

хо

#### Author(s)

Madeleine Cule

Robert Gramacy

Richard Samworth

## See Also

dmarglcd, mlelcd

mlelcd

Compute the maximum likelihood estimator of a log-concave density

## **Description**

Uses Shor's r-algorithm to compute the maximum likelihood estimator of a log-concave density based on an i.i.d. sample. The estimator is uniquely determined by its value at the data points. The output is an object of class "LogConcDEAD" which contains all the information needed to plot the estimator using the plot method, or to evaluate it using the function dlcd.

## Usage

```
mlelcd(x, w=rep(1/nrow(x),nrow(x)), y=initialy(x),
  verbose=-1, alpha=5, c=1, sigmatol=10^-8, integraltol=10^-4,
  ytol=10^-4, Jtol=0.001, chtol=10^-6)
```

#### **Arguments**

Data in  $R^d$ , in the form of an  $n \times d$  numeric matrix

We Vector of weights  $w_i$  such that the computed estimator maximizes

$$\sum_{i=1}^{n} w_i \log f(x_i)$$

subject to the restriction that f is log-concave. The default is  $\frac{1}{n}$  for all i, which corresponds to i.i.d. observations.

Vector giving starting point for the r-algorithm. If none given, a kernel estimate is used.

verbose • -1: (default) prints nothing • 0: prints warning messages • n > 0: prints summary information every n iterations Scalar parameter for SolvOpt alpha Scalar giving starting step size Real-valued scalar giving one of the stopping criteria: Relative change in  $\sigma$  must sigmatol be below sigmatol for algorithm to terminate. (See Details) Real-valued scalar giving on of the stopping criteria: Relative change in y must ytol be below ytol for algorithm to terminate. (See Details) integraltol Real-valued scalar giving one of the stopping criteria:  $|1 - \exp(\bar{h}_y)|$  must be below integral to l for algorithm to terminate. (See Details) Parameter controlling when Taylor expansion is used in computing the function Jtol chtol Parameter controlling convex hull computations

#### **Details**

The log-concave maximum likelihood density estimator based on data  $X_1, \ldots, X_n$  is the function that maximizes

$$\sum_{i=1}^{n} w_i \log f(X_i)$$

subject to the constraint that f is log-concave. For i.i.d.~data, the weights  $w_i$  should be  $\frac{1}{n}$  for each i.

This is a function of the form  $\bar{h}_y$  for some  $y \in \mathbb{R}^n$ , where

$$\bar{h}_y(x) = \inf\{h(x) : h \text{ concave }, h(x_i) \ge y_i \text{ for } i = 1, \dots, n\}.$$

Functions of this form may equivalently be specified by dividing  $C_n$ , the convex hull of the data, into simplices  $C_j$  for  $j \in J$  (triangles in 2d, tetrahedra in 3d etc.), and setting

$$f(x) = \exp\{b_j^T x - \beta_j\}$$

for  $x \in C_i$ , and f(x) = 0 for  $x \notin C_n$ .

This function uses Shor's r-algorithm (an iterative subgradient-based procedure) to minimize over vectors y in  $\mathbb{R}^n$  the function

$$\sigma(y) = -\frac{1}{n} \sum_{i=1}^{n} y_i + \int \exp(\bar{h}_y(x)) dx.$$

This is equivalent to finding the log-concave maximum likelihood estimator, as demonstrated in Cule, Samworth and Stewart (2008).

An implementation of Shor's r-algorithm based on **SolvOpt** is used.

Computing  $\sigma$  makes use of the **qhull** library. Code from this C-based library is copied here as it is not currently possible to use compiled code from another library. For points not in general position, this requires a Taylor expansion of  $\sigma$ , discussed in *Cule and Duembgen (2008)*.

#### Value

An object of class "LogConcDEAD", with the following components:

x Data copied from input (may be reordered)

weights copied from input (may be reordered)

logMLE vector of the log of the maximum likelihood estimate, evaluated at the obser-

vation points

NumberOfEvaluations

Vector containing the number of steps, number of function evaluations, and

number of subgradient evaluations. If the SolvOpt algorithm fails, the first com-

ponent will be an error code (< 0).

MinSigma Real-valued scalar giving minimum value of the objective function

b matrix containing row by row the values of  $b_i$ 's corresponding to each triangu-

lation; see also the Details section above

beta vector containing the values of  $\beta_j$ 's corresponding to each triangulation; see

also the Details section above

triang matrix containing final triangulation of the convex hull of the data

verts matrix containing details of triangulation for use in dlcd vertsoffset matrix containing details of triangulation for use in dlcd

chull Vector containing vertices of faces of the convex hull of the data

outnorm matrix where each row is an outward pointing normal vectors for the faces of

the convex hull of the data. The number of vectors depends on the number of

faces of the convex hull.

outoffset matrix where each row is a point on a face of the convex hull of the data. The

number of vectors depends on the number of faces of the convex hull.

## Note

For one-dimensional data, the active set algorithm of logcondens is faster, and may be preferred.

The authors gratefully acknowledge the assistance of Lutz Duembgen at the University of Bern for his insight into the objective function  $\sigma$ .

Further references, including definitions and background material, may be found in *Cule*, *Samworth* and *Stewart* (2010).

#### Author(s)

Madeleine Cule

Robert B. Gramacy

Richard Samworth

Yining Chen

#### References

Barber, C.B., Dobkin, D.P., and Huhdanpaa, H.T. (1996) *The Quickhull algorithm for convex hulls* ACM Trans. on Mathematical Software, 22(4) p.469-483 http://www.qhull.org

Cule, M. L. and Duembgen, L. (2008) On an auxiliary function for log-density estimation, University of Bern technical report. https://arxiv.org/abs/0807.4719

Cule, M. L., Samworth, R. J., and Stewart, M. I. (2010) *Maximum likelihood estimation of a log-concave density*, Journal of the Royal Statistical Society, Series B, 72(5) p.545-607.

Kappel, F. and Kuntsevich, A. V. (2000) *An implementation of Shor's r-algorithm*, Computational Optimization and Applications, Volume 15, Issue 2, 193-205.

Shor, N. Z. (1985) Minimization methods for nondifferentiable functions, Springer-Verlag

#### See Also

```
logcondens, interplcd, plot.LogConcDEAD, interpmarglcd, rlcd, dlcd, dmarglcd, cov.LogConcDEAD
```

#### **Examples**

```
## Some simple normal data, and a few plots
x <- matrix(rnorm(200),ncol=2)</pre>
lcd <- mlelcd(x)</pre>
g <- interplcd(lcd)</pre>
oldpar <- par(mfrow = c(1,1))
par(mfrow=c(2,2), ask=TRUE)
plot(lcd, g=g, type="c")
plot(lcd, g=g, type="c", uselog=TRUE)
plot(lcd, g=g, type="i")
plot(lcd, g=g, type="i", uselog=TRUE)
par(oldpar)
## 2D interactive plot (need rgl package, not run here)
if(interactive()) {plot(lcd, type="r")}
## Some plots of marginal estimates
g.marg1 <- interpmarglcd(lcd, marg=1)</pre>
g.marg2 <- interpmarglcd(lcd, marg=2)</pre>
plot(lcd, marg=1, g.marg=g.marg1)
plot(lcd, marg=2, g.marg=g.marg2)
## generate some points from the fitted density
## via independent rejection sampling
generated1 <- rlcd(100, lcd)</pre>
colMeans(generated1)
## via Metropolis-Hastings algorithm
generated2 <- rlcd(100, lcd, "MH")</pre>
colMeans(generated2)
```

22 plot.LogConcDEAD

```
## evaluate the fitted density
mypoint <- c(0, 0)
dlcd(mypoint, lcd, uselog=FALSE)
mypoint \leftarrow c(1, 0)
dlcd(mypoint, lcd, uselog=FALSE)
## evaluate the marginal density
dmarglcd(0, lcd, marg=1)
dmarglcd(1, lcd, marg=2)
## evaluate the covariance matrix of the fitted density
covariance <- cov.LogConcDEAD(lcd)</pre>
## find the hat matrix for the smoothed log-concave that
## matches empirical mean and covariance
A <- hatA(lcd)
## evaluate the fitted smoothed log-concave density
mypoint <- c(0, 0)
dslcd(mypoint, lcd, A)
mypoint <- c(1, 0)
dslcd(mypoint, lcd, A)
## generate some points from the fitted smoothed log-concave density
generated <- rslcd(100, lcd, A)</pre>
```

plot.LogConcDEAD

Plot a log-concave maximum likelihood estimator

## Description

plot method for class "LogConcDEAD". Plots of various types are available for 1- and 2-d data. For dimension greater than 1, plots of axis-aligned marginal density estimates are available.

#### Usage

```
## S3 method for class 'LogConcDEAD'
plot(x, uselog=FALSE, type="ic", addp=TRUE,
    drawlabels=TRUE, gridlen=400, g, marg, g.marg, main, xlab, ylab, ...)
```

## **Arguments**

X	Object of class "LogConcDEAD" (typically output from mlelcd)
uselog	Scalar logical: should the plot be on the log scale?
type	Plot type: "p" perspective, "c" contour, "i" image, ic image and contour, r using <b>rgl</b> (the best!)
addp	Scalar logical: should the data points be plotted? (as black dots on the surface for $d \ge 2$ ; as circles for $d = 1$ )

plot.LogConcDEAD 23

drawlabels	Scalar logical: should labels be added to contour lines? (only relevant for types "ic" and "c")
gridlen	Integer scalar indicating the number of points at which the maximum likelihood estimator is evaluated in each dimension
g	(optional) a matrix of density estimate values (the result of a call to interplcd). If many plots of a single dataset are required, it may be quicker to compute the grid using interplcd(x) and pass the result to plot
marg	If non-NULL, this scalar integer determines which marginal should be plotted (should be between $1\ \mathrm{and}\ d)$
g.marg	If g is non-NULL, can contain a vector of marginal density estimate values (the output of interpmarglcd). If many plots of a single dataset are required, it may be quicker to compute the marginal values to compute marginal values using interpmarglcd and pass the result to plot
main	Title
xlab	x-axis label
ylab	y-axis label
	Other arguments to be passed to the generic plot method

#### **Details**

The density estimate is evaluated on a grid of points using the interplcd function. If several plots are required, this may be computed separately and passed to plot using the g argument.

For two dimensional data, the default plot type is "ic", corresponding to image and contour plots. These may be obtained separately using plot type "i" or "c" respectively. Where available, the use of plot type "r" is recommended. This uses the **rgl** package to produce a 3-d plot that may be rotated by the user. The option "p" produces perspective plots.

For data of dimension at least 2, axis-aligned marginals may be plotted by setting the marg argument. This integrates the estimated density over the remaining dimensions. If several plots are required, the estimate may be computed using the function interpmarglcd and passed using the argument g.marg.

Where relevant, the colors were obtained from the function heat\_hcl in the colorspace package. Thanks to Achim Zeileis for this suggestion.

For examples, see mlelcd.

#### Value

No return value, plot will display

#### Author(s)

Madeleine Cule Robert B. Gramacy Richard Samworth Yining Chen

print.LogConcDEAD

#### See Also

mlelcd, interplcd, interpmarglcd, heat\_hcl

print.LogConcDEAD

Summarizing log-concave maximum likelihood estimator

## **Description**

Generic print and summary method for objects of class "LogConcDEAD"

#### Usage

```
## S3 method for class 'LogConcDEAD'
print(x, ...)
## S3 method for class 'LogConcDEAD'
summary(object, ...)
```

## Arguments

X	Object of class "LogConcDEAD" (typically output from mlelcd), as required by print
object	Object of class "LogConcDEAD" (typically output from mlelcd), as required by summary
	Other arguments passed to print or summary

#### **Details**

print and summary currently perform the same function.

If there has been an error computing the maximum likelihood estimator, an error message is printed. Otherwise, the value of the log maximum likelihood estimator at observation points is printed. The number of interations required by the subgradient and the number of function evaluations are also

printed.

#### Value

No return value, log MLE at observation points will be printed out on the screen.

## Author(s)

```
Madeleine Cule
Robert B. Gramacy
Richard Samworth
```

#### See Also

mlelcd

rlcd 25

rlcd	Sample from a log-concave maximum likelihood estimate

#### **Description**

Draws samples from a log-concave maximum likelihood estimate. The estimate should be specified in the form of an object of class "LogConcDEAD", the result of a call to mlelcd.

## Usage

```
rlcd(n=1, lcd, method=c("Independent","MH"))
```

#### **Arguments**

n A scalar integer indicating the number of samples required

lcd Object of class "LogConcDEAD" (typically output from mlelcd)

method Indicator of the method used to draw samples, either via independent rejection

campling (dafault choice) or via Matropolic Hactings

sampling (default choice) or via Metropolis-Hastings

#### **Details**

This function by default uses a simple rejection sampling scheme to draw independent random samples from a log-concave maximum likelihood estimator. One can also use the Metropolis-Hastings option to draw (dependent) samples with a higher acceptance rate.

For examples, see mlelcd.

#### Value

A numeric matrix with nsample rows, each row corresponding to a point in  $\mathbb{R}^d$  drawn from the distribution with density defined by lcd.

#### Note

Details of the rejection sampling can be found in Appendix B.3 of *Cule, Samworth and Stewart* (2010). Details of the Metropolis-Hastings scheme can be found in *Gopal and Casella* (2010)

## Author(s)

Yining Chen

Madeleine Cule

Robert Gramacy

Richard Samworth

26 rslcd

#### References

Cule, M. L., Samworth, R. J., and Stewart, M. I. (2010) *Maximum likelihood estimation of a multi-dimensional log-concave density* J. Roy. Statist. Soc., Ser. B. (with discussion), 72, 545-600.

Gopal, V. and Casella, G. (2010) Discussion of Maximum likelihood estimation of a log-concave density by Cule, Samworth and Stewart J. Roy. Statist. Soc., Ser. B., 72, 580-582.

#### See Also

mlelcd

rslcd

Sample from a smoothed log-concave maximum likelihood estimate

## Description

Draws samples from a smoothed log-concave maximum likelihood estimate. The estimate should be specified in the form of an object of class "LogConcDEAD", the result of a call to mlelcd, and a positive definite matrix.

#### Usage

```
rslcd(n=1, lcd, A=hatA(lcd), method=c("Independent","MH"))
```

## **Arguments**

n	A scalar integer indicating the number of samples required
lcd	Object of class "LogConcDEAD" (typically output from mlelcd)
A	A positive definite matrix that determines the degree of smoothing, typically taken as the output of hat A(1cd) $$
method	Indicator of the method used to draw samples, either via independent rejection sampling (default choice) or via Metropolis-Hastings

## **Details**

This function by default uses a simple rejection sampling scheme to draw independent random samples from a smoothed log-concave maximum likelihood estimator. One can also use the Metropolis-Hastings option to draw (dependent) samples with a higher acceptance rate.

For examples, see mlelcd.

## Value

A numeric matrix with n rows, each row corresponding to a point in  $\mathbb{R}^d$  drawn from the distribution with density defined by 1cd and A.

rslcd 27

#### Author(s)

Yining Chen

Madeleine Cule

Robert Gramacy

Richard Samworth

## References

Chen, Y. and Samworth, R. J. (2013) *Smoothed log-concave maximum likelihood estimation with applications* Statist. Sinica, 23, 1373-1398. https://arxiv.org/abs/1102.1191v4

Cule, M. L., Samworth, R. J., and Stewart, M. I. (2010) *Maximum likelihood estimation of a multi-dimensional log-concave density* J. Roy. Statist. Soc., Ser. B. (with discussion), 72, 545-600.

Gopal, V. and Casella, G. (2010) Discussion of Maximum likelihood estimation of a log-concave density by Cule, Samworth and Stewart J. Roy. Statist. Soc., Ser. B., 72, 580-582.

#### See Also

mlelcd, rlcd, hatA

# **Index**

* EM	rlcd, 25
EMmixlcd, 9	rslcd, 26
* classification	* nonparametric
EMmixlcd, 9	cov.LogConcDEAD,4
interactive2D, 15	dlcd, 5
* datagen	dmarglcd,7
rlcd, 25	dslcd, 8
rslcd, 26	EMmixlcd, 9
* distribution	getinfolcd, 11
dlcd, 5	getweights, 13
rlcd, 25	hatA, 14
rslcd, 26	interactive2D, 15
* dplot	interplcd, 16
dmarglcd, 7	interpmarglcd, 17
interplcd, 16	LogConcDEAD-package, 2
interpmarglcd, 17	mlelcd, 18
plot.LogConcDEAD, 22	plot.LogConcDEAD, 22
* dynamic	print.LogConcDEAD, 24
plot.LogConcDEAD, 22	rlcd, 25
* hplot	rslcd, 26
plot.LogConcDEAD, 22	* package
* iplot	LogConcDEAD-package, 2
plot.LogConcDEAD, 22	* smoothing
* multivariate	dslcd, 8
cov.LogConcDEAD, 4	hatA, 14
dlcd, 5	LogConcDEAD-package, 2
dmarglcd, 7	rslcd, 26
dslcd, 8	contour, 16, 23
EMmixlcd, 9	cov.LogConcDEAD, 4, 15, 21
getinfolcd, 11	., 10, 21
getweights, 13	dlcd, 2, 5, 9, 10, 12, 18, 20, 21
hatA, 14	dmarglcd, 3, 7, 18, 21
interactive2D, 15	dslcd, 3, 8, 16
interplcd, 16	
interpmarglcd, 17	EMmixlcd, 9
LogConcDEAD-package, 2	getinfolcd, 11
mlelcd, 18	getweights, 13
plot.LogConcDEAD, 22	getweights, 13
print.LogConcDEAD, 24	hatA, 2, 5, 9, 14, 27
	, , , , , , ,

INDEX 29

```
heat_hcl, 24
image, 16, 23
interactive2D, 15
interplcd, 3, 16, 21, 23, 24
interpmarglcd, 3, 17, 21, 23, 24
LogConcDEAD (LogConcDEAD-package), 2
LogConcDEAD-package, 2
logcondens, 3, 4, 8, 10, 20, 21
mclust, 10
mlelcd, 2, 3, 5-14, 16-18, 18, 22-27
plot, 18, 22, 23
plot.LogConcDEAD, 3, 10, 16, 17, 21, 22
print, 3
print.LogConcDEAD, 24
rgl, 4, 22, 23
rlcd, 3, 21, 25, 27
rslcd, 3, 26
summary, 3
\verb|summary.LogConcDEAD||
         (print.LogConcDEAD), 24
tkrplot, 15
```