Package ‘fdadensity’

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Type Package

Title Functional Data Analysis for Density Functions by Transformation to a Hilbert Space

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Description An implementation of the methodology described in Petersen and Mueller (2016) <doi:10.1214/15-AOS1363> for the functional data analysis of samples of density functions. Densities are first transformed to their corresponding log quantile densities, followed by ordinary Functional Principal Components Analysis (FPCA). Transformation modes of variation yield improved interpretation of the variability in the data as compared to FPCA on the densities themselves. The standard fraction of variance explained (FVE) criterion commonly used for functional data is adapted to the transformation setting, also allowing for an alternative quantification of variability for density data through the Wasserstein metric of optimal transport.

Depends R (>= 3.3.0)

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LazyData false

Imports Rcpp (>= 0.11.5), fdapace (>= 0.3.0)

LinkingTo Rcpp

NeedsCompilation yes

Suggests testthat

RoxygenNote 7.0.2

Encoding UTF-8

Repository CRAN

Date/Publication 2019-12-05 06:20:02 UTC
Description

The approximate kernel density estimates of the 813 bacterial organisms’ isoelectric point (pI) protein distributions.

Format

A matrix with 813 rows and 768 columns:

- **rowname**: General organism identifier
- **colspace**: pH in [0,14]

References

The authors would like to thank Dr. Chris Knight for providing the original data.
CreateModeOfVarPlotLQ2D

Transformation Mode of Variation Plot

Description

Create the k-th transformation mode of variation plot.

Usage

CreateModeOfVarPlotLQ2D(
  fpcaObj, 
  domain = "D", 
  k = 1, 
  dSup = NULL, 
  Qvec = -2:2, 
  alpha = 0, 
  useAlpha = FALSE, 
  ... 
)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>fpcaObj</td>
<td>An FPCA class object returned by FPCA() on the log quantile density functions.</td>
</tr>
<tr>
<td>domain</td>
<td>should the mode be plotted in LQD ('Q') or density space ('D', the default).</td>
</tr>
<tr>
<td>k</td>
<td>The k-th mode of variation to plot (default k = 1)</td>
</tr>
<tr>
<td>dSup</td>
<td>The common support of the original densities. Only relevant for domain = 'D'</td>
</tr>
<tr>
<td>Qvec</td>
<td>Vector of values Q to be plotted. If 0 is not included, it will be added (default is -2:2). Only relevant for domain = 'D'</td>
</tr>
<tr>
<td>alpha</td>
<td>(De)regularisation parameter (default is 0). See details.</td>
</tr>
<tr>
<td>useAlpha</td>
<td>logical - should deregularisation be performed? Default:FALSE</td>
</tr>
<tr>
<td>...</td>
<td>Additional arguments for the 'plot' function.</td>
</tr>
</tbody>
</table>

Details

If domain = 'D' (the default), the a transformation mode of variation is plotted. The red-line is \( \psi^{-1}(\nu) \), where \( \nu \) is the mean in LQD space and \( \psi \) is the LQD transformation. Other lines correspond to perturbations by adding multiples of the LQD eigenfunctions \( \rho_k \) (with eigenvalues \( \tau_k \)): \( \psi^{-1}(\nu + Q \sqrt{\tau_k} \rho_k) \) for the values \( Q \) in Qvec. If alpha is positive, will attempt to deregularise (see DeregulariseByAlpha). This will throw an error if alpha is too large.

If domain = 'Q', ordinary modes of variation are plotted in LQD space (see documentation for CreateModeOfVarPlot in fdapace).
References


See Also

DeregulariseByAlpha

Examples

## Densities for Top 50 Male Baby Names
data(Top50BabyNames)
x = Top50BabyNames$x

# Perform Transformation FPCA for male baby name densities
X = FPCAdens(dmatrix = t(Top50BabyNames$dens$male), dSup = Top50BabyNames$x, useAlpha = TRUE, optns = list(dataType = "Dense", error = FALSE, methodSelectK = 2))

# Plot Modes
Qvec = quantile(X$xiEst[,1], probs = c(0.1, 0.25, 0.75, 0.9))/sqrt(X$lambda[1])
CreateModeOfVarPlotLQ2D(X, k = 1, dSup = x, Qvec = Qvec, main = 'First Mode, Density Space')
CreateModeOfVarPlotLQ2D(X, domain = 'Q', k = 1, dSup = x, Qvec = Qvec, main = 'First Mode, LQD space')

Qvec = quantile(X$xiEst[,2], probs = c(0.1, 0.25, 0.75, 0.9))/sqrt(X$lambda[2])
CreateModeOfVarPlotLQ2D(X, k = 2, dSup = x, Qvec = Qvec, main = 'Second Mode, Density Space')
CreateModeOfVarPlotLQ2D(X, domain = 'Q', k = 2, dSup = x, Qvec = Qvec, main = 'Second Mode, LQD space')

dens2lqd
Function for converting densities to log quantile density functions

Description

Function for converting densities to log quantile density functions

Usage

dens2lqd(dens, dSup, N = length(dSup), lqdSup = NULL)

Arguments

dens
density values on dSup - must be strictly positive and integrate to 1
dSup
support (grid) for Density domain
N
desired number of points on a [0,1] grid for lqd function; default length(dSup)
lqdSup
support for lqd domain - must begin at 0 and end at 1; default [0,1] with N-equidistant support points
**dens2qd**

**Value**

lqd log quantile density on lqdSup

**References**

*Functional Data Analysis for Density Functions by Transformation to a Hilbert space, Alexander Petersen and Hans-Georg Mueller, 2016*

**See Also**

`normaliseDensities`

**Examples**

```r
x <- seq(0,2,length.out =512)
y <- rep(0.5,length.out =512)
y.lqd <- dens2lqd( dens=y, dSup = x) # should equate # log(2)
```

**dens2qd**

*Function for converting Densities to Quantile Densities*

**Description**

Function for converting Densities to Quantile Densities

**Usage**

```r
dens2qd( 
  dens, 
  dSup = seq(0, 1, length.out = length(dens)), 
  qdSup = seq(0, 1, length.out = length(dens)), 
  useSplines = TRUE
)
```

**Arguments**

- `dens`: density on dSup
- `dSup`: support for Density domain - max and min values mark the boundary of the support.
- `qdSup`: support for quantile density domain - must begin at 0 and end at 1
- `useSplines`: fit spline to the qd when doing the numerical integration (default: TRUE)

**Value**

qd quantile density values on qdSup
dens2quantile

Function for converting Densities to Quantile Functions

Usage

dens2quantile(
  dens,
  dSup = seq(0, 1, length.out = length(dens)),
  qSup = seq(0, 1, length.out = length(dens)),
  useSplines = TRUE
)

Arguments

dens density on dSup
dSup support for Density domain - max and min values mark the boundary of the support.
qSup support for quantile domain - must begin at 0 and end at 1
useSplines fit spline to the qd when doing the numerical integration (default: TRUE)

Value

Q quantile function on qSup

References

DeregulariseByAlpha

See Also

normaliseDensities

Examples

```r
x <- seq(0,2,length.out =512)
y <- rep(0.5,length.out =512)
y.quantile <- dens2quantile(dens=y, dSup = x) # should equate # 2*seq(0, 1, length.out = 512)
```

---

**DeregulariseByAlpha**  
*Function to deregularise densities to have (smaller) minimum value*

---

**Description**

If possible, deregularises the input density \( y \) to have minimum density value is \( \alpha \). See details.

**Usage**

```r
DeregulariseByAlpha(x, y, alpha = 0)
```

**Arguments**

- `x`: support of the density
- `y`: values of the density
- `alpha`: scalar to deregularise with (default = 0) - this will be the minimum value of the deregularised density, unless \( \min(y) < \alpha \), in which case no deregularisation will be performed

**Details**

If \( \min(y) \leq \alpha \), or \( y \) is the uniform distribution, no deregularisation is performed and \( y \) is returned. If \( \min(y) \times \text{diff(range}(x)) > 1 \), the deregularisation is not possible and an error is thrown. Otherwise, the deregularised density in an inverse manner to RegulariseByAlpha.

**Value**

- `dens`: density values on \( x \)

**See Also**

RegulariseByAlpha
Examples

```r
x = seq(0,1,length.out=122)
y = seq(0.1,1.9,length.out=122)
z = DeregulariseByAlpha(x=x, y=y, alpha = 0)
```

FPCAdens  
FPCA for densities by log quantile density transformation

Description

Perform FPCA on LQD-transformed densities

Usage

```r
FPCAdens(
  dmatrix,
  dSup,
  lqdSup = seq(0, 1, length.out = length(dSup)),
  useAlpha = FALSE,
  alpha = 0.01,
  optns = list(dataType = "Dense", error = FALSE)
)
```

Arguments

- `dmatrix`: Matrix holding the density values on dSup - all rows must be strictly positive and integrate to 1
- `dSup`: Support (grid) for Density domain
- `lqdSup`: Support grid for lqd domain (default = seq(0, 1, length.out = length(dSup)))
- `useAlpha`: should regularisation be performed (default=FALSE)
- `alpha`: Scalar to regularise the supports with (default=0.01)
- `optns`: A list of options for FPCA. See documentation for FPCA.

Details

Densities are transformed to log-quantile densities, followed by standard FPCA. If `useAlpha = TRUE`, densities are regularized before transformation

References

*Functional Data Analysis for Density Functions by Transformation to a Hilbert space, Alexander Petersen and Hans-Georg Mueller, 2016*
See Also

RegulariseByAlpha, lqd2dens, MakeLQDsample, FPCA

Examples

```r
## Densities for Top 50 Female Baby Names
data(Top50BabyNames)

# Perform Transformation FPCA for male baby name densities
X = FPCAdens(dmatrix = t(Top50BabyNames$dens$female), dSup = Top50BabyNames$x, useAlpha = TRUE,
   optns = list(dataType = 'Dense', error = FALSE, methodSelectK = 2))

x = Top50BabyNames$x

# Plot Modes
Qvec = quantile(X$xiEst[,1], probs = c(0.1, 0.25, 0.75, 0.9))/sqrt(X$lambda[1])
CreateModeOfVarPlotLQ2D(X, k = 1, dSup = x, Qvec = Qvec, main = 'First Mode, Density space')
CreateModeOfVarPlotLQ2D(X, domain = 'Q', k = 1, dSup = x, Qvec = Qvec,
   main = 'First Mode, LQD space')

Qvec = quantile(X$xiEst[,2], probs = c(0.1, 0.25, 0.75, 0.9))/sqrt(X$lambda[2])
CreateModeOfVarPlotLQ2D(X, k = 2, dSup = x, Qvec = Qvec, main = 'Second Mode, Density Space')
CreateModeOfVarPlotLQ2D(X, domain = 'Q', k = 2, dSup = x, Qvec = Qvec,
   main = 'Second Mode, LQD space')
```

### GetFVE

**Compute Metric-based Fraction of Variance Explained**

**Description**

When FPCA is performed on the log quantile density functions, the fraction of variance explained by the first K components is computed based on the density reconstruction and chosen metric.

**Usage**

```r
GetFVE(fpcaObj, dmatrix, dSup, metric = "L2", useAlpha = FALSE, alpha = 0.01)
```

**Arguments**

- `fpcaObj` PACE output (FPCA on LQDs)
- `dmatrix` matrix of original densities measures on grid dSup, rows correspond to individual densities
- `dSup` support for Density domain - max and min mark the boundary of the support
- `metric` metric for measuring variance - 'L2' for Euclidean or 'W' for Wasserstein
- `useAlpha` should regularisation be performed to densities in dmatrix? This should be set to TRUE if densities were regularised prior to FPCA (default = FALSE)
alpha  scalar to regularise before computing FVE. If useAlpha = TRUE, this should match the value used to regularise prior to FPCA (default = 0.01)

Details

The fraction of variance explained (FVE) by the first K principal components corresponding to the LQD functions is computed by taking the K-dimensional LQD representations, transforming back to densities, and comparing the reconstruction to the original densities using the chosen metric. If densities were regularised prior to transformation and FPCA, the same regularisation parameters should be used here.

Value

FVEvector

References

*Functional Data Analysis for Density Functions by Transformation to a Hilbert space, Alexander Petersen and Hans-Georg Mueller, 2016*

See Also

RegulariseByAlpha,lqd2quantile

Examples

data(Top50BabyNames)

# Perform Transformation FPCA for male baby name densities
dSup = Top50BabyNames$x
X = FPCAdens(dmatrix = t(Top50BabyNames$dens$male), dSup = dSup, useAlpha = TRUE,
          optns = list(dataType = 'Dense', error = FALSE, methodSelectK = 8))

# Compute FVE - must compare to regularized densities
fveL2 = GetFVE(fpcaObj = X, dmatrix = t(Top50BabyNames$dens$male), dSup = dSup, useAlpha = TRUE)
fveW = GetFVE(fpcaObj = X, dmatrix = t(Top50BabyNames$dens$male), dSup = dSup,
             metric = 'W', useAlpha = TRUE)

---

getWFmean  \textit{Wasserstein Frechet Mean Computation}

Description

Function for computing the Wasserstein Frechet mean through quantile density averaging
Usage

```r
getWFmean(
  dmatrix,
  dSup,
  N = length(dSup),
  qdSup = seq(0, 1, length.out = N),
  useAlpha = FALSE,
  alpha = 0.01
)
```

Arguments

- `dmatrix`: matrix of density values on `dSup` - must be strictly positive and each row must integrate to 1
- `dSup`: support (grid) for Density domain
- `N`: desired number of points on a [0,1] grid for quantile density functions; default `length(dSup)`
- `qdSup`: support for LQ domain - must begin at 0 and end at 1; default [0,1] with `N`-equidistant support points
- `useAlpha`: should regularisation be performed (default=FALSE)
- `alpha`: Scalar to regularise the supports with (default=0.01)

Value

`wfmean` the Wasserstein-Frechet mean density

References

*Functional Data Analysis for Density Functions by Transformation to a Hilbert space, Alexander Petersen and Hans-Georg Mueller, 2016*

Examples

```r
x <- seq(0,1,length.out = 101)
# linear densities on (0, 1)
y <- t(sapply(seq(0.5, 1.5, length.out = 10), function(b) b + 2*(1 - b)*x))
wfmean = getWFmean(y, x)

# Plot WF mean with Euclidean Mean
matplot(x, t(y), ylab = 'Density', type = 'l', lty = 1, col = 'black')
lines(x, wfmean, lwd = 2, col = 'red')
lines(x, colMeans(y), lwd = 2, col = 'blue')
legend('topright', col = c('black', 'red', 'blue'), lwd = c(1, 2, 2),
       legend = c('Densities', 'WF Mean', 'Euclidean Mean'))
```
**lqd2dens**

*Function for converting log quantile densities to densities*

**Description**

Function for converting log quantile densities to densities

**Usage**

```r
lqd2dens(
  lqd,
  lqdSup = seq(0, 1, length.out = length(lqd)),
  dSup,
  useSplines = TRUE
)
```

**Arguments**

- `lqd`: log quantile density on lqdSup
- `lqdSup`: support for lqd domain - must begin at 0 and end at 1
- `dSup`: support for Density domain - max and min values mark the boundary of the support.
- `useSplines`: fit spline to the lqd when doing the numerical integration (default: TRUE)

**Value**

dens density values on dSup

**References**

*Functional Data Analysis for Density Functions by Transformation to a Hilbert space, Alexander Petersen and Hans-Georg Mueller, 2016*

**Examples**

```r
x <- seq(0, 2, length.out = 512)
y.lqd <- rep(log(2), times = 512)
y <- lqd2dens(dSup=x, lqd = y.lqd) # should equate # 1/2
```
**lqd2quantile**  
*Function for converting log quantile densities to quantile functions*

**Description**
Function for converting log quantile densities to quantile functions

**Usage**
```r
lqd2quantile(
  lqd,
  lqdSup = seq(0, 1, length.out = length(lqd)),
  lb = 0,
  useSplines = TRUE
)
```

**Arguments**
- **lqd**: log quantile density on lqdSup
- **lqdSup**: support for lqd domain - must begin at 0 and end at 1
- **lb**: lower bound of support for Density domain - default is 0.
- **useSplines**: fit spline to the lqd when doing the numerical integration (default: TRUE)

**Value**
quantile values on lqdSup

**References**
*Functional Data Analysis for Density Functions by Transformation to a Hilbert space, Alexander Petersen and Hans-Georg Mueller, 2016*

**Examples**
```r
x <- seq(1, 3, length.out = 512)
y.lqd <- rep(log(2), times = 512)
y <- lqd2quantile(lqd = y.lqd, lb = 1)  # should equate # seq(1, 3, length.out = 512)
```
Description

See 'lqd2dens' and 'DeregulariseByAlpha' for more details. This function transforms the log quantile densities in 'qmatrix' to density functions, optionally followed by deregularisation.

Usage

MakeDENsample(
  qmatrix,
  lqdSup = seq(0, 1, length.out = ncol(qmatrix)),
  dSup = seq(0, 1, length.out = ncol(qmatrix)),
  useAlpha = FALSE,
  alpha = 0
)

Arguments

qmatrix  Matrix holding the log quantile density values on [0,1]
lqdSup   Support grid for input log quantile densities (default = seq(0, 1, length.out = ncol(qmatrix)))
dSup     Support grid for output densities (default = seq(0, 1, length.out = ncol(qmatrix)))
useAlpha Logical indicator to deregularise the densities (default = FALSE)
alpha    Scalar to deregularise the density - where possible, this will be the minimum value for the deregularised densities (default=0)

Value

list with the 'DEN' transformed data, and 'dSup' that matches the input argument.

References


See Also

DeregulariseByAlpha,lqd2dens
Examples

```r
x <- seq(0,1,length.out = 101)
# linear densities on (0, 1)
y <- t(sapply(seq(0.5, 1.5, length.out = 10), function(b) b + 2*(1 - b)*x))  
# Get LQDs
y.lqd = MakeLQDsample(dmatrix = y, dSup = x)  
matplot(y.lqd$lqdSup, t(y.lqd$LQD), ylab = 'LQD', type = 'l', lty = 1, col = 'black')

# Get Densities Back
y.dens = MakeDENsample(y.lqd$LQD, lqdSup = x, dSup = x) # should equate to y above
# These should look the same
matplot(y.dens$dSup, t(y.dens$DEN), ylab = 'Density', type = 'l', lty = 1, col = 'blue')
matplot(x, t(y), ylab = 'Original Density', type = 'l', lty = 1, col = 'red')
```

---

**MakeLQDsample**  
Convenience function for converting densities to log-quantile densities

**Description**

See 'dens2lqd' and 'RegulariseByAlpha' for more details. This function first (transforms the densities in 'dmatrix' to log quantile density functions, optionally followed by regularisation.

**Usage**

```r
MakeLQDsample(
  dmatrix,  
dSup,  
lqdSup = seq(0, 1, length.out = length(dSup)),  
useAlpha = FALSE,  
alpha = 0.01  
)
```

**Arguments**

- **dmatrix**: Matrix holding the density values on dSup - all rows must be strictly positive and integrate to 1  
- **dSup**: Support (grid) for Density domain  
- **lqdSup**: Support grid for lqd domain (default = seq(0, 1, length.out = length(dSup)))  
- **useAlpha**: should regularisation be performed (default=FALSE)  
- **alpha**: Scalar to regularise the supports with (default=0.01)
normaliseDensities

Value

list with 'LQD', a matrix of log quantile density functions, and 'lqdSup' that matches the input argument

References

*Functional Data Analysis for Density Functions by Transformation to a Hilbert space, Alexander Petersen and Hans-Georg Mueller, 2016*

See Also

RegulariseByAlpha, dens2lqd

Examples

```r
x <- seq(0,1,length.out = 101)
# some log quantile densities on (0, 1)
y <- t(sapply(seq(0.5, 1.5, length.out = 10), function(b) -log(b^2 + 4*(1-b)*x)/2))
# Get densities
y.dens = MakeDENsample(qmatrix = y, lqdSup = x, dSup = x)$DEN
matplot(x, t(y.dens), ylab = 'Density', type = 'l', lty = 1, col = 'black')
# Get LQDs Back
y.lqd = MakeLQDsample(y.dens, lqdSup = x, dSup = x)
# These should match
matplot(y.lqd$lqdSup, t(y.lqd$LQD), ylab = 'LQD', type = 'l', lty = 1, col = 'blue')
matplot(x, t(y), ylab = 'LQD', type = 'l', lty = 1, col = 'red')
```

normaliseDensities Normalise Densities

Description

Preprocessing function to ensure densities integrate to 1

Usage

```r
normaliseDensities(dmatrix, dSup = 1:ncol(dmatrix))
```

Arguments

dmatrix Matrix with rows representing distinct densities on dSup - all entries must be nonnegative
dSup Support (grid) for Density domain
qd2dens

Details

Uses trapezoidal integration to normalise the densities to have integral 1

Value

matrix 'dmatrix' consisting of rows of input of the same name that have been normalised to have integral 1

References


Examples

## Normalise collection of truncated normal densities

```r
mu <- seq(-2, 2, by = 0.5)
dSup = seq(-3, 3, length.out = 101)
y <- t(sapply(mu, function(m) dnorm(x = dSup, mean = m)))

# Should return warnings about densities not integrating to 1
lqd = MakeLQDsample(dmatrix = y, dSup = dSup)

# Normalise and rerun without warning
dens <- normaliseDensities(dmatrix = y, dSup = dSup)
lqd = MakeLQDsample(dmatrix = dens, dSup = dSup)
```

qd2dens Function for converting Quantile Densities to Densities

Description

Function for converting Quantile Densities to Densities

Usage

```r
qd2dens(
  qd,
  qdSup = seq(0, 1, length.out = length(qd)),
  dSup,
  useSplines = TRUE
)
```
RegulariseByAlpha

Arguments

qd quantile density on qdSup
qdSup support for quantile domain - must begin at 0 and end at 1 (default = seq(0, 1, length.out = length(qd)))
dSup support for Density domain - max and min values mark the boundary of the support.
useSplines fit spline to the qd when doing the numerical integration (default: TRUE)

Value
dens density values on dSup

References

*Functional Data Analysis for Density Functions by Transformation to a Hilbert space, Alexander Petersen and Hans-Georg Mueller, 2016*

Examples

```r
x <- seq(0, 1, length.out = 512)
y <- rep(2, length.out = 512)
y.dens <- qd2dens(qd = y, qdSup = x, dSup = seq(0, 2, length.out = 512)) # should equate ≈ 1/2
```

RegulariseByAlpha Function to regularise densities to have (larger) minimum value

Description

If possible, regularises the input density \( y \) to have minimum density value is \( \alpha \). See details.

Usage

`RegulariseByAlpha(x, y, alpha = 0.01)`

Arguments

\( x \) support of the density
\( y \) values of the density
\( \alpha \) scalar to regularise with (default = 0.01) - this will be the minimum value of the regularised density, unless \( \min(y) > \alpha \), in which case no regularisation will be performed
Details

If \( \min(y) \geq \alpha \) or \( y \) is the uniform distribution, no regularisation is performed and \( y \) is returned. If \( \alpha \cdot \text{diff}(\text{range}(x)) > 1 \), the regularisation is not possible and an error is thrown. Otherwise, the regularised density is computed by adding an appropriate constant \( \gamma \), followed by renormalisation to have integral 1.

Value

dens density values on \( x \)

See Also

DeregulariseByAlpha, normaliseDensities

Examples

\[
\begin{align*}
x &= \text{seq}(0,1,\text{length.out}=122) \\
y &= \text{seq}(0,2,\text{length.out}=122) \\
z &= \text{RegulariseByAlpha}(x=x, y=y, \alpha = 0.1)
\end{align*}
\]

Description

Baby name popularity densities, obtained by smoothing year-to-year popularity indices from 1950 to 2016, after normalization to have integral equal to 1. The top 50 names, in absolute popularity, are included for each gender.

Format

A list with two variables

- \( x \) grid of years between 1950 and 2016, of length 67.
- \( \text{dens} \) list of length two, corresponding to male (\( \text{dens}\$\text{male} \)) and female (\( \text{dens}\$\text{female} \)) names. Each is a 67-by-50 matrix of density estimates, where each column corresponds to a unique baby name given by the corresponding column name.

References

Data from the R package babynames, originally from the US Social Security Administration
Index

BacteriaPI, 2
CreateModeOfVarPlotLQ2D, 3

dens2lqd, 4, 16
dens2qd, 5
dens2quantile, 6
DeregulariseByAlpha, 4, 7, 14, 19

FPCA, 9
FPCAdens, 8

GetFVE, 9
gWFmean, 10

lqd2dens, 9, 12, 14
lqd2quantile, 10, 13

MakeDENsample, 14
MakeLQDsample, 9, 15

normaliseDensities, 5–7, 16, 19
qd2dens, 17

RegulariseByAlpha, 7, 9, 10, 16, 18
Top50BabyNames, 19