Package 'polykde'

February 17, 2025

Type Package

Title Polyspherical Kernel Density Estimation

```
Version 1.0.0
Date 2025-02-13
Description Kernel density estimation on the polysphere, hypersphere, and
     circle. Includes functions for density estimation, regression estimation,
     ridge estimation, bandwidth selection, kernels, samplers, and homogeneity
     tests. Companion package to García-Portugués and Meilán-Vila (2024)
     <doi:10.48550/arXiv.2411.04166> and García-Portugués and Meilán-Vila
     (2023) <doi:10.1007/978-3-031-32729-2_4>.
License GPL-3
Imports abind, doFuture, foreach, future, gsl, movMF, progressr, Rcpp
     (>= 1.0.8.3), RcppProgress, rotasym, sphunif
Suggests alphashape3d, DirStats, FixedPoint, ks, manipulate, numDeriv,
     optimParallel, testthat, viridis, rgl, scatterplot3d, sdetorus,
     smacof
LinkingTo Rcpp, RcppArmadillo, RcppProgress
URL https://github.com/egarpor/polykde
BugReports https://github.com/egarpor/polykde/issues
Encoding UTF-8
RoxygenNote 7.3.2
NeedsCompilation yes
Author Eduardo García-Portugués [aut, cre]
       (<https://orcid.org/0000-0002-9224-4111>),
     Andrea Meilán-Vila [ctb] (<a href="https://orcid.org/0000-0001-8537-9280">https://orcid.org/0000-0001-8537-9280</a>)
Maintainer Eduardo García-Portugués <edgarcia@est-econ.uc3m.es>
Repository CRAN
Date/Publication 2025-02-17 11:00:01 UTC
```

2 Contents

Contents

Index

olykde-package	 3
ngles_to_polysph	 3
ngles_to_sph	4
ngles_to_torus	 5
w_cv_kre_polysph	 6
w_cv_polysph	 7
w_lcv_min_epa	 8
w_mrot_polysph	 9
w_rot_polysph	 10
lean_euler_ridge	 11
omp_ind_dj	 12
urv_vmf_polysph	 13
ist_polysph	 14
_unif_polysph	 15
_vmf_polysph	 16
ff_kern	 16
uler_ridge	 18
rad_hess_kde_polysph	20
om_test_polysph	 22
ndex_ridge	 24
nterp_polysph	 26
de_polysph	 27
ernel	 28
re_polysph	 29
og_cv_kde_polysph	 30
olylog_minus_exp_mu	 31
roj_grad_kde_polysph	 32
roj_polysph	 33
_g_kern	 34
_kde_polysph	 35
_kern_polysph	 36
_path_s1r	 38
_unif_polysph	 40
_vmf_polysph	 41
oftplus	 42
iew_srep	 42

44

polykde-package 3

polykde-package polykde: Polyspherical Kernel Density Estimation

Description

Kernel density estimation on the polysphere, hypersphere, and circle. Includes functions for density estimation, regression estimation, ridge estimation, bandwidth selection, kernels, samplers, and homogeneity tests. Companion package to García-Portugués and Meilán-Vila (2024) <doi:10.48550/arXiv.2411.04166> and García-Portugués and Meilán-Vila (2023) <doi:10.1007/978303132729-2_4>.

Author(s)

Eduardo García-Portugués.

References

García-Portugués, E. and Meilán-Vila, A. (2024). Kernel density estimation with polyspherical data and its applications. *arXiv*:2411.04166. doi:10.48550/arXiv.2411.04166.

García-Portugués, E. and Meilán-Vila, A. (2023). Hippocampus shape analysis via skeletal models and kernel smoothing. In Larriba, Y. (Ed.), *Statistical Methods at the Forefront of Biomedical Advances*, pp. 63–82. Springer, Cham. doi:10.1007/9783031327292_4.

See Also

Useful links:

- https://github.com/egarpor/polykde
- Report bugs at https://github.com/egarpor/polykde/issues

 ${\it angles_to_polysph} \qquad {\it Conversion \ between \ the \ angular \ and \ Cartesian \ coordinates \ of \ the \ polysphere}$

Description

Obtain the angular coordinates of points on a polysphere $S^{d_1} \times \cdots \times S^{d_r}$, and vice versa.

Usage

```
angles_to_polysph(theta, d)
polysph_to_angles(x, d)
```

4 angles_to_sph

Arguments

theta	matrix of size c(n, sum(d)) with the angles.
d	vector with the dimensions of the polysphere.
X	matrix of size c(n, sum(d + 1)) with the Cartesian coordinates on $\mathcal{S}^{d_1} \times \cdots \times$
	\mathcal{S}^{d_r} . Assumed to be of unit norm by blocks of coordinates in the rows.

Value

- angles_to_polysph: the matrix x.
- polysph_to_angles: the matrix theta.

Examples

```
# Check changes of coordinates polysph_to_angles(angles_to_polysph(rep(pi / 2, 3), d = 2:1), d = 2:1) angles_to_polysph(polysph_to_angles(x = c(0, 0, 1, 0, 1), d = 2:1), d = 2:1)
```

angles_to_sph

Conversion between the angular and Cartesian coordinates of the hypersphere

Description

```
Transforms the angles (\theta_1, \dots, \theta_d) in [0, \pi)^{d-1} \times [-\pi, \pi) into the Cartesian coordinates (\cos(x_1), \sin(x_1)\cos(x_2), \dots, \sin(x_1)\cdots\sin(x_{d-1})\cos(x_d), \sin(x_1)\cdots\sin(x_{d-1})\sin(x_d)) of the hypersphere \mathcal{S}^d, and vice versa.
```

Usage

```
angles_to_sph(theta)
sph_to_angles(x)
```

Arguments

theta matrix of size c(n, d) with the angles. x matrix of size c(n, d + 1) with the Cartesian coordinates on S^d . Assumed to be of unit norm by rows.

Value

- angles_to_sph: the matrix x.
- sph_to_angles: the matrix theta.

angles_to_torus 5

Examples

angles_to_torus

Conversion between the angular and Cartesian coordinates of the torus

Description

Transforms the angles $(\theta_1, \dots, \theta_d)$ in $[-\pi, \pi)^d$ into the Cartesian coordinates

$$(\cos(x_1), \sin(x_1), \dots, \cos(x_d), \sin(x_d))$$

of the torus $(S^1)^d$, and vice versa.

Usage

```
angles_to_torus(theta)
torus_to_angles(x)
```

Arguments

theta matrix of size c(n, d) with the angles. x matrix of size c(n, 2*d) with the Cart

matrix of size c(n, 2 * d) with the Cartesian coordinates on $(S^1)^d$. Assumed to be of unit norm by pairs of coordinates in the rows.

Value

- angles_to_torus: the matrix x.
- torus_to_angles: the matrix theta.

```
# Check changes of coordinates
torus_to_angles(angles_to_torus(c(0, pi / 3, pi / 2)))
torus_to_angles(angles_to_torus(rbind(c(0, pi / 3, pi / 2), c(0, 1, -2))))
angles_to_torus(torus_to_angles(c(0, 1, 1, 0)))
angles_to_torus(torus_to_angles(rbind(c(0, 1, 1, 0), c(0, 1, 0, 1))))
```

6 bw_cv_kre_polysph

bw_cv_kre_polysph	al-on-scalar re-
-------------------	------------------

Description

Computes least squares cross-validation bandwidths for kernel regression estimation with polyspherical response and scalar predictor. It computes both the bandwidth that minimizes the cross-validation loss and its "one standard error" variant.

Usage

```
bw_cv_kre_polysph(X, Y, d, p = 0, h_grid = bw.nrd(X) * 10^seq(-2, 2, l = 100), plot_cv = TRUE, fast = TRUE)
```

Arguments

Χ	a vector of size n with the predictor sample.
Υ	a matrix of size $c(n, sum(d) + r)$ with the response sample on the polysphere.
d	vector of size r with dimensions.
p	degree of local fit, either 0 or 1. Defaults to 0.
h_grid	bandwidth grid where to optimize the cross-validation loss. Defaults to bw. $nrd(X) * 10^seq(-1, 1, 1 = 100)$.
plot_cv	plot the cross-validation loss curve? Defaults to TRUE.
fast	use the faster and equivalent version of the cross-validation loss? Defaults to TRUE.

Details

A similar output to glmnet's cv.glmnet is returned.

Value

A list with the following fields:

h_min	the bandwidth that minimizes the cross-validation loss.
h_1se	the largest bandwidth within one standard error of the minimal cross-validation loss.
cvm	the mean of the cross-validation loss curve.
cvse	the standard error of the cross-validation loss curve.

bw_cv_polysph 7

Examples

```
n <- 50
X <- seq(0, 1, 1 = n)
Y <- r_path_s2r(n = n, r = 1, sigma = 0.1, spiral = TRUE)[, , 1]
bw_cv_kre_polysph(X = X, Y = Y, d = 2, p = 0)
bw_cv_kre_polysph(X = X, Y = Y, d = 2, p = 1, fast = FALSE)</pre>
```

bw_cv_polysph Cross-validation bandwidth selection for polyspherical kernel density estimator

Description

Likelihood Cross-Validation (LCV) and Least Squares Cross-Validation (LSCV) bandwidth selection for the polyspherical kernel density estimator.

Usage

```
bw_cv_polysph(X, d, kernel = 1, kernel_type = 1, k = 10,
type = c("LCV", "LSCV")[1], M = 10000, bw0 = NULL, na.rm = FALSE,
ncores = 1, h_min = 0, upscale = FALSE, deriv = 0, ...)
```

Arguments

Χ	a matrix of size $c(n, sum(d) + r)$ with the sample.
d	vector of size r with dimensions.
kernel	kernel employed: 1 for von Mises–Fisher (default); 2 for Epanechnikov; 3 for softplus.
kernel_type	type of kernel employed: 1 for product kernel (default); 2 for spherically symmetric kernel.
k	softplus kernel parameter. Defaults to 10.0.
type	cross-validation type, either "LCV" (default) or "LSCV".
М	Monte Carlo samples to use for approximating the integral in the LSCV loss.
bw0	initial bandwidth for minimizing the CV loss. If NULL, it is computed internally by magnifying the $bw_rot_polysph$ bandwidths by 50%.
na.rm	remove NAs in the objective function? Defaults to FALSE.
ncores	number of cores used during the optimization. Defaults to 1.
h_min	minimum h enforced (componentwise). Defaults to \emptyset .
upscale	rescale the resulting bandwidths to work for derivative estimation? Defaults to $\ensuremath{FALSE}.$
deriv	derivative order to perform the upscaling. Defaults to \emptyset .
• • •	further arguments passed to optim(if ncores = 1) or optimParallel (if ncores > 1).

8 bw_lcv_min_epa

Value

A list as optim or optimParallel output. In particular, the optimal bandwidth is stored in par.

Examples

bw_lcv_min_epa

Minimum bandwidth allowed in likelihood cross-validation for Epanechnikov kernels

Description

This function computes the minimum bandwidth allowed in likelihood cross-validation with Epanechnikov kernels, for a given dataset and dimension.

Usage

```
bw_lcv_min_epa(X, d, kernel_type = c("prod", "sph")[1])
```

Arguments

X a matrix of size c(n, sum(d) + r) with the sample.

d vector of size r with dimensions.

kernel_type type of kernel employed: 1 for product kernel (default); 2 for spherically sym-

metric kernel.

Value

The minimum bandwidth allowed.

```
n <- 5
d <- 1:3
X <- r_unif_polysph(n = n, d = d)
h_min <- rep(bw_lcv_min_epa(X = X, d = d), length(d))
log_cv_kde_polysph(X = X, d = d, h = h_min - 1e-4, kernel = 2) # Problem
log_cv_kde_polysph(X = X, d = d, h = h_min + 1e-4, kernel = 2) # OK</pre>
```

bw_mrot_polysph 9

bw_mrot_polysph	bw_mrot_polysph	
-----------------	-----------------	--

Description

Computes marginal (sphere by sphere) rule-of-thumb bandwidths for the polyspherical kernel density estimator using a von Mises–Fisher distribution as reference.

Usage

```
bw_mrot_polysph(X, d, kernel = 1, k = 10, upscale = FALSE, deriv = 0,
   kappa = NULL, ...)
```

Arguments

Χ	a matrix of size $c(n, sum(d) + r)$ with the sample.
d	vector of size r with dimensions.
kernel	kernel employed: 1 for von Mises–Fisher (default); 2 for Epanechnikov; 3 for softplus.
k	softplus kernel parameter. Defaults to 10.0.
upscale	rescale bandwidths to work on $\mathcal{S}^{d_1} \times \cdots \times \mathcal{S}^{d_r}$ and for derivative estimation? Defaults to FALSE. If upscale = 1, the order n is upscaled. If upscale = 2, then also the kernel constant is upscaled.
deriv	derivative order to perform the upscaling. Defaults to \emptyset .
kappa	estimate of the concentration parameters. Computed if not provided (default).
• • •	further arguments passed to nlm.

Value

A vector of size r with the marginal optimal bandwidths.

bw_rot_polysph

bw_rot_polysph	Rule-of-thumb bandwidth selection for polyspherical kernel density estimator
----------------	------------------------------------------------------------------------------

Description

Computes the rule-of-thumb bandwidth for the polyspherical kernel density estimator using a product of von Mises–Fisher distributions as reference in the Asymptotic Mean Integrated Squared Error (AMISE).

Usage

```
bw_rot_polysph(X, d, kernel = 1, kernel_type = c("prod", "sph")[1],
bw0 = NULL, upscale = FALSE, deriv = 0, k = 10, kappa = NULL, ...)
```

Arguments

Χ	a matrix of size c(n, sum(d) + r) with the sample.
d	vector of size r with dimensions.
kernel	kernel employed: 1 for von Mises–Fisher (default); 2 for Epanechnikov; 3 for softplus.
kernel_type	type of kernel employed: 1 for product kernel (default); 2 for spherically symmetric kernel.
bw0	initial bandwidth for minimizing the CV loss. If NULL, it is computed internally by magnifying the bw_mrot_polysph bandwidths by 50%.
upscale	rescale bandwidths to work on $\mathcal{S}^{d_1} \times \cdots \times \mathcal{S}^{d_r}$ and for derivative estimation? Defaults to FALSE. If upscale = 1, the order n is upscaled. If upscale = 2, then also the kernel constant is upscaled.
deriv	derivative order to perform the upscaling. Defaults to 0.
k	softplus kernel parameter. Defaults to 10.0.
kappa	estimate of the concentration parameters. Computed if not provided (default).
	further arguments passed to nlm.

Details

The selector assumes that the density curvature matrix R of the unknown density is approximable by that of a product of von Mises-Fisher densities, $R(\kappa)$. The estimation of the concentration parameters κ is done by maximum likelihood.

Value

A list with entries bw (optimal bandwidth) and opt, the latter containing the output of nlm.

clean_euler_ridge 11

Examples

clean_euler_ridge

Clean ridge points coming from spurious fits

Description

Remove points from the ridge that are spurious. The cleaning is done by removing end points in the Euler algorithm that did not converge, do not have a negative second eigenvalue, or are in low-density regions.

Usage

```
clean_euler_ridge(e, X, p_out = NULL)
```

Arguments

```
e outcome from euler_ridge or parallel_euler_ridge.

X a matrix of size c(n, sum(d) + r) with the sample.

p_out proportion of outliers to remove. Defaults to NULL (no cleaning).
```

Value

A list with the same structure as that returned by euler_ridge, but with the spurious points. The removed points are informed in the removed field.

12 comp_ind_dj

```
h_rid <- 0.5
h_{eu} \leftarrow h_{rid^2}
N <- 30
eps <- 1e-6
X0 \leftarrow r_unif_polysph(n = n, d = d)
Y \leftarrow euler\_ridge(x = X0, X = X, d = d, h = h\_rid, h\_euler = h\_eu,
                  N = N, eps = eps, keep_paths = TRUE)
Y_removed <- clean_euler_ridge(e = Y, X = X)$removed
col_X[Y_removed] <- 2</pre>
col_X_alp[Y_removed] <- 2</pre>
# Visualization
i <- N \# Between 1 and N
sc3 <- scatterplot3d::scatterplot3d(Y$paths[, , 1], color = col_X_alp,</pre>
                                       pch = 19, xlim = c(-1, 1),
                                       ylim = c(-1, 1), zlim = c(-1, 1),
                                       xlab = "x", ylab = "y", zlab = "z")
sc3$points3d(rbind(Y$paths[, , i]), col = col_X, pch = 16, cex = 0.75)
for (k in seq_len(nrow(Y$paths))) {
  sc3$points3d(t(Y$paths[k, , ]), col = col_X_alp[k], type = "1")
}
```

comp_ind_dj

Index of hyperspheres on a polysphere

Description

Given Cartesian coordinates of polyspherical data, computes the 0-based indexes at which the Cartesian coordinates for each hypersphere start and end.

Usage

```
comp_ind_dj(d)
```

Arguments

d

vector of size r with dimensions.

Value

A vector of size sum(d) + 1.

```
# Example on (S^1)^3
d <- c(1, 1, 1)
comp_ind_dj(d = d)
comp_ind_dj(d = d) + 1
```

curv_vmf_polysph 13

```
# Example on S^1 x S^2

d \leftarrow c(1, 2)

comp_ind_dj(d = d)

comp_ind_dj(d = d) + 1
```

curv_vmf_polysph

Curvature of a polyspherical von Mises–Fisher density

Description

Computes the curvature matrix $R(\kappa)$ of a product of von Mises-Fisher densities on the polysphere. This curvature is used in the rule-of-thumb selector bw_rot_polysph.

Usage

```
curv_vmf_polysph(kappa, d, log = FALSE)
```

Arguments

kappa a vector of size r with the von Mises–Fisher concentrations.

d vector of size r with dimensions.

log compute the (entrywise) logarithm of the curvature matrix? Defaults to FALSE.

Value

A matrix of size c(length(r), length(r)).

14 dist_polysph

dist_polysph

Polyspherical distance

Description

Computation of the distance between points x and y on the polysphere $S^{d_1} \times \cdots \times S^{d_r}$:

$$\sqrt{\sum_{j=1}^r d_{\mathcal{S}^{d_j}}(\boldsymbol{x}_j,\boldsymbol{y}_j)^2},$$

where $d_{\mathcal{S}^{d_j}}(\boldsymbol{x}_j, \boldsymbol{y}_j) = \cos^{-1}(\boldsymbol{x}_i' \boldsymbol{y}_j)$

Usage

```
dist_polysph(x, y, ind_dj, norm_x = FALSE, norm_y = FALSE, std = TRUE)
dist_polysph_cross(x, y, ind_dj, norm_x = FALSE, norm_y = FALSE,
    std = TRUE)
dist_polysph_matrix(x, ind_dj, norm_x = FALSE, norm_y = FALSE,
    std = TRUE)
```

Arguments

```
x a matrix of size c(n, sum(d) + r). 
y either a matrix of size c(m, sum(d) + r) or a vector of length sum(d) + r. 
ind_dj   0-based index separating the blocks of spheres that is computed with comp_ind_dj. 
norm_x, norm_y ensure a normalization of the data? Default to FALSE. 
standardize distance to [0,1]? Uses that the maximum distance is \sqrt{r}\pi. Defaults to TRUE.
```

Value

- dist_polysph: a vector of size n with the distances between x and y.
- dist_polysph_matrix: a matrix of size c(n, n) with the pairwise distances of x.
- dist_polysph_cross: a matrix of distances of size c(n, m) with the cross distances between x and y.

```
# Example on S^2 x S^3 x S^1
d <- c(2, 3, 1)
ind_dj <- comp_ind_dj(d)
n <- 3
x <- r_unif_polysph(n = n, d = d)</pre>
```

d_unif_polysph 15

```
y <- r_unif_polysph(n = n, d = d)

# Distances of x to y
dist_polysph(x = x, y = y, ind_dj = ind_dj, std = FALSE)
dist_polysph(x = x, y = y[1, , drop = FALSE], ind_dj = ind_dj, std = FALSE)

# Pairwise distance matrix of x
dist_polysph_matrix(x = x, ind_dj = ind_dj, std = FALSE)

# Cross distances between x and y
dist_polysph_cross(x = x, y = y, ind_dj = ind_dj, std = FALSE)</pre>
```

d_unif_polysph

Density of the uniform distribution on the polysphere

Description

Computes the density of the uniform distribution on the polysphere.

Usage

```
d_{unif_polysph(x, d, log = FALSE)}
```

Arguments

x a matrix of size c(nx, sum(d) + r) with the evaluation points.

d vector of size r with dimensions.

log compute the logarithm of the density? Defaults to FALSE.

Value

A vector of size nx with the evaluated density.

```
# Simple check of integration on S^1 x S^2 d \leftarrow c(1, 2) x \leftarrow r_unif_polysph(n = 1e4, d = d) mean(1 / d_unif_polysph(x = x, d = d)) / prod(rotasym::w_p(p = d + 1))
```

16 eff_kern

	Density of the product of von Mises–Fisher distributions on the polysphere
--	----------------------------------------------------------------------------

Description

Computes the density of the product of von Mises–Fisher densities on the polysphere.

Usage

```
d_vmf_polysph(x, d, mu, kappa, log = FALSE)
```

Arguments

х	a matrix of size $c(nx, sum(d) + r)$ with the evaluation points.
d	vector of size r with dimensions.
mu	a vector of size sum(d) + r with the concatenated von Mises-Fisher means.
kappa	a vector of size r with the von Mises-Fisher concentrations.
log	compute the logarithm of the density? Defaults to FALSE.

Value

A vector of size nx with the evaluated density.

Examples

```
# Simple check of integration on S^1 x S^2 d \leftarrow c(1, 2) mu \leftarrow c(0, 1, 0, 1, 0) kappa \leftarrow c(1, 1) x \leftarrow r_vmf_polysph(n = 1e4, d = d, mu = mu, kappa = kappa) mean(1 / d_vmf_polysph(x = x, d = d, mu = mu, kappa = kappa)) / prod(rotasym::w_p(p = d + 1))
```

eff_kern

Polyspherical kernel moments and efficiencies

Description

Computes moments of kernels on $\mathcal{S}^{d_1} \times \cdots \times \mathcal{S}^{d_r}$ and efficiencies of kernels on $(\mathcal{S}^d)^r$.

eff_kern 17

Usage

```
eff_kern(d, r, k = 10, kernel, kernel_type = c("prod", "sph")[1],
    kernel_ref = "2", kernel_ref_type = c("prod", "sph")[2], ...)

b_d(kernel, d, k = 10, kernel_type = c("prod", "sph")[1], ...)

v_d(kernel, d, k = 10, kernel_type = c("prod", "sph")[1], ...)
```

Arguments

d a scalar with the common dimension of each hypersphere S^d . a scalar with the number of polyspheres of the same dimension. r k softplus kernel parameter. Defaults to 10.0. kernel kernel employed: 1 for von Mises–Fisher (default); 2 for Epanechnikov; 3 for softplus. kernel_type type of kernel. Must be either "prod" (product kernel, default) or "sph" (spherically symmetric kernel). kernel_ref reference kernel to which compare the efficiency. Uses the same codification as the kernel. Defaults to "2". kernel_ref_type type of the reference kernel. Must be either "prod" (product kernel) or "sph" (spherically symmetric kernel, default). further arguments passed to integrate, such as upper, abs.tol, rel.tol, etc.

Value

- b_d: a vector with the first kernel moment on each hypersphere (common if kernel_type = "sph").
- v_d: a vector with the second kernel moment if kernel_type = "prod", or a scalar if kernel_type = "snh"
- eff_kern: a scalar with the kernel efficiency.

```
# Kernel moments
b_d(kernel = 2, d = c(2, 3), kernel_type = "prod")
v_d(kernel = 2, d = c(2, 3), kernel_type = "prod")
b_d(kernel = 2, d = c(2, 3), kernel_type = "sph")
v_d(kernel = 2, d = c(2, 3), kernel_type = "sph")

# Kernel efficiencies
eff_kern(d = 2, r = 1, kernel = "1")
eff_kern(d = 2, r = 1, kernel = "2")
eff_kern(d = 2, r = 1, k = 10, kernel = "3")
```

18 euler_ridge

-			
eu	er	ridge	

Euler algorithms for polyspherical density ridge estimation

Description

Functions to perform density ridge estimation on the polysphere $S^{d_1} \times \cdots \times S^{d_r}$ through the Euler algorithm in standard, parallel, or block mode.

Usage

```
euler_ridge(x, X, d, h, h_euler = as.numeric(c()),
    weights = as.numeric(c()), wrt_unif = FALSE, normalized = TRUE,
    norm_x = FALSE, norm_X = FALSE, kernel = 1L, kernel_type = 1L,
    k = 10, N = 1000L, eps = 1e-05, keep_paths = FALSE,
    proj_alt = TRUE, fix_u1 = TRUE, sparse = FALSE, show_prog = TRUE,
    show_prog_j = FALSE)

parallel_euler_ridge(x, X, d, h, h_euler, N = 1000, eps = 1e-05,
    keep_paths = FALSE, cores = 1, ...)

block_euler_ridge(x, X, d, h, h_euler, ind_blocks, N = 1000, eps = 1e-05,
    keep_paths = FALSE, cores = 1, ...)
```

Arguments

х	a matrix of size $c(nx, sum(d) + r)$ with the starting points for the Euler algorithm.
Χ	a matrix of size $c(n, sum(d) + r)$ with the sample.
d	vector of size r with dimensions.
h	vector of size r with bandwidths.
h_euler	vector of size r with the advance steps in the Euler method. Set internally as h if not provided.
weights	weights for each observation. If provided, a vector of size n with the weights for multiplying each kernel. If not provided, set internally to $rep(1 / n, n)$, which gives the standard estimator.
wrt_unif	flag to return a density with respect to the uniform measure. If FALSE (default), the density is with respect to the Lebesgue measure.
normalized	flag to compute the normalizing constant of the kernel and include it in the kernel density estimator. Defaults to TRUE.
norm_x, norm_X	ensure a normalization of the data? Defaults to FALSE.
kernel	kernel employed: 1 for von Mises–Fisher (default); 2 for Epanechnikov; 3 for softplus.
kernel_type	type of kernel employed: 1 for product kernel (default); 2 for spherically symmetric kernel.

euler_ridge 19

k softplus kernel parameter. Defaults to 10.0.

N maximum number of Euler iterations. Defaults to 1e3.

eps convergence tolerance. Defaults to 1e-5.

keep_paths keep the Euler paths to the ridge? Defaults to FALSE.

proj_alt alternative projection. Defaults to TRUE.

fix_u1 ensure the u_1 vector is different from x? Prevents the Euler algorithm to "surf

the ridge". Defaults to TRUE.

sparse use a sparse eigendecomposition of the Hessian? Defaults to FALSE.

show_prog display a progress bar for x? Defaults to TRUE. show_prog_j display a progress bar for N? Defaults to FALSE.

cores cores to use. Defaults to 1.

... further arguments passed to euler_ridge.
ind_blocks indexes of the blocks, a vector or length r.

Details

euler_ridge is the main function to perform density ridge estimation through the Euler algorithm from the starting values x to initiate the ridge path. The function euler_ridge_parallel parallelizes on the starting values x. The function euler_ridge_block runs the Euler algorithm marginally in blocks of hyperspheres, instead of jointly in the whole polysphere. This function requires that all the dimensions are the same.

Value

The three functions return a list with the following fields:

ridge_y a matrix of size c(nx, sum(d) + r) with the end points of Euler algorithm defin-

ing the estimated ridge.

lamb_norm_y a matrix of size c(nx, sum(d) + r) with the Hessian eigenvalues (largest to

smallest) evaluated at end points.

log_dens_y a column vector of size c(nx, 1) with the logarithm of the density at end points.

paths an array of size c(nx, sum(d) + r, N + 1) containing the Euler paths.

start_x a matrix of size c(nx, sum(d) + r) with the starting points for the Euler algo-

rithm.

iter a column vector of size c(nx, 1) counting the iterations required for each point.

conv a column vector of size c(nx, 1) with convergence flags.

d vector d.

bandwidth used for the kernel density estimator.

error a column vector of size c(nx, 1) indicating if errors were found for each path.

Examples

```
## Test on S^2 with a small circle trend
# Sample
r <- 1
d <- 2
n <- 50
ind_dj \leftarrow comp_ind_dj(d = d)
set.seed(987204452)
X < -r_{path_s2r(n = n, r = r, spiral = FALSE, Theta = cbind(c(1, 0, 0)),
                 sigma = 0.35)[, , 1]
col_X_alp <- viridis::viridis(n, alpha = 0.25)</pre>
col_X <- viridis::viridis(n)</pre>
# Euler
h_rid <- 0.5
h_{eu} \leftarrow h_{rid^2}
N <- 30
eps <- 1e-6
Y \leftarrow euler\_ridge(x = X, X = X, d = d, h = h\_rid, h\_euler = h\_eu,
                  N = N, eps = eps, keep_paths = TRUE)
# Visualization
i <- N # Between 1 and N
sc3 <- scatterplot3d::scatterplot3d(Y$paths[, , 1], color = col_X_alp,</pre>
                                      pch = 19, xlim = c(-1, 1),
                                      ylim = c(-1, 1), zlim = c(-1, 1),
                                      xlab = "x", ylab = "y", zlab = "z")
sc3$points3d(rbind(Y$paths[, , i]), col = col_X, pch = 16, cex = 0.75)
for (k in seq_len(nrow(Y$paths))) {
  sc3$points3d(t(Y$paths[k, , ]), col = col_X_alp[k], type = "1")
}
```

grad_hess_kde_polysph Gradient and Hessian of the polyspherical kernel density estimator

Description

Computes the gradient $D\hat{f}(x; h)$ and Hessian matrix $H\hat{f}(x; h)$ of the kernel density estimator $\hat{f}(x; h)$ on the polysphere $S^{d_1} \times \cdots \times S^{d_r}$.

Usage

```
grad_hess_kde_polysph(x, X, d, h, weights = as.numeric(c()),
    projected = TRUE, proj_alt = TRUE, norm_grad_hess = FALSE,
    log = FALSE, wrt_unif = FALSE, normalized = TRUE, norm_x = FALSE,
    norm_X = FALSE, kernel = 1L, kernel_type = 1L, k = 10)
```

Arguments

X	a matrix of size $c(nx, sum(d) + r)$ with the evaluation points.
Χ	a matrix of size $c(n, sum(d) + r)$ with the sample.
d	vector of size r with dimensions.
h	vector of size r with bandwidths.
weights	weights for each observation. If provided, a vector of size n with the weights for multiplying each kernel. If not provided, set internally to rep(1 / n , n), which gives the standard estimator.
projected	compute the $projected$ gradient and Hessian that accounts for the radial projection? Defaults to TRUE.
proj_alt	alternative projection. Defaults to TRUE.
norm_grad_hess	normalize the gradient and Hessian dividing by the kernel density estimator? Defaults to FALSE.
log	compute the logarithm of the density? Defaults to FALSE.
wrt_unif	flag to return a density with respect to the uniform measure. If $FALSE$ (default), the density is with respect to the Lebesgue measure.
normalized	flag to compute the normalizing constant of the kernel and include it in the kernel density estimator. Defaults to TRUE.
norm_x, norm_X	ensure a normalization of the data? Defaults to FALSE.
kernel	kernel employed: 1 for von Mises–Fisher (default); 2 for Epanechnikov; 3 for softplus.
kernel_type	type of kernel employed: 1 for product kernel (default); 2 for spherically symmetric kernel.
k	softplus kernel parameter. Defaults to 10.0.

Value

A list with the following components:

dens a column vector of size c(nx, 1) with the kernel density estimator evaluated at

х.

grad a matrix of size c(nx, sum(d) + r) with the gradient of the kernel density esti-

mator evaluated at x.

hess an array of size c(nx, sum(d) + r, sum(d) + r) with the Hessian matrix of the

kernel density estimator evaluated at x.

```
# Simple check on (S^1)^2

n <- 3

d <- c(1, 1)

mu <- c(0, 1, 0, 1)

kappa <- c(5, 5)

h <- c(0.2, 0.2)
```

22 hom_test_polysph

```
X \leftarrow r\_vmf\_polysph(n = n, d = d, mu = mu, kappa = kappa) grh \leftarrow grad\_hess\_kde\_polysph(x = X, X = X, d = d, h = h) str(grh) grh
```

hom_test_polysph

Homogeneity test for several polyspherical samples

Description

Permutation tests for the equality of distributions of two or k samples of data on $\mathcal{S}^{d_1} \times \cdots \times \mathcal{S}^{d_r}$. The Jensen–Shannon distance is used to construct a test statistic measuring the discrepancy between the k kernel density estimators. Tests based on the mean and scatter matrices are also available, but for only two samples (k=2).

Usage

```
hom_test_polysph(X, d, labels, type = c("jsd", "mean", "scatter", "hd")[1],
h = NULL, kernel = 1, kernel_type = 1, k = 10, B = 1000,
M = 10000, plot_boot = FALSE, seed_jsd = NULL, cv_jsd = TRUE)
```

Arguments

guments	
Χ	a matrix of size $c(n, sum(d) + r)$ with the sample.
d	vector of size r with dimensions.
labels	vector with k different levels indicating the group.
type	kind of test to be performed: "jsd" (default), a test comparing the kernel density estimators for k groups using the Jensen–Shannon distance; "mean", a simple test for the equality of two means (non-omnibus for testing homogeneity); "scatter", a simple test for the equality of two scatter matrices; "hd", a test comparing the kernel density estimators for two groups using the Hellinger distance.
h	vector of size r with bandwidths.
kernel	kernel employed: 1 for von Mises-Fisher (default); 2 for Epanechnikov; 3 for softplus.
kernel_type	type of kernel employed: 1 for product kernel (default); 2 for spherically symmetric kernel.
k	softplus kernel parameter. Defaults to 10.0.
В	number of permutations to use. Defaults to 1e3.
М	number of Monte Carlo replicates to use when approximating the Hellinger/Jensen-Shannon distance. Defaults to 1e4.
plot_boot	flag to display a graphical output of the test decision. Defaults to FALSE.
seed_jsd	seed for the Monte Carlo simulations used to estimate the integrals in the Jensen–Shannon distance.
cv_jsd	use cross-validation to approximate the Jensen-Shannon distance? Does not

require Monte Carlo. Defaults to TRUE.

hom_test_polysph 23

Details

```
Only type = "jsd" is able to deal with k > 2.
```

The "jsd" statistic is the Jensen-Shannon divergence. This statistic is bounded in [0,1]. The "mean" statistic measures the maximum (chordal) distance between the estimated group means. This statistic is bounded in [0,1]. The "scatter" statistic measures the maximum affine invariant Riemannian metric between the estimated scatter matrices. The "hd" statistic computes a monotonic transformation of the Hellinger distance, which is the Bhattacharyya divergence (or coefficient).

Value

An object of class "htest" with the following fields:

statistic the value of the test statistic. p.value the p-value of the test. statistic_perm the B permuted statistics. a table with the sample sizes per group. h bandwidths used. В number of permutations. alternative a character string describing the alternative hypothesis. method the kind of test performed. a character string giving the name of the data. data.name

```
## Two-sample case
# H0 holds
n < -c(50, 100)
X1 \leftarrow rotasym::r_vMF(n = n[1], mu = c(0, 0, 1), kappa = 1)
X2 \leftarrow rotasym::r_vMF(n = n[2], mu = c(0, 0, 1), kappa = 1)
hom_test_polysph(X = rbind(X1, X2), labels = rep(1:2, times = n),
                  d = 2, type = "jsd", h = 0.5)
# H0 does not hold
X2 \leftarrow rotasym::r_vMF(n = n[2], mu = c(0, 1, 0), kappa = 2)
hom_test_polysph(X = rbind(X1, X2), labels = rep(1:2, times = n),
                  d = 2, type = "jsd", h = 0.5)
## k-sample case
# H0 holds
n < -c(50, 100, 50)
X1 \leftarrow rotasym::r_vMF(n = n[1], mu = c(0, 0, 1), kappa = 1)
X2 \leftarrow rotasym::r_vMF(n = n[2], mu = c(0, 0, 1), kappa = 1)
X3 \leftarrow rotasym::r_vMF(n = n[3], mu = c(0, 0, 1), kappa = 1)
hom_test_polysph(X = rbind(X1, X2, X3), labels = rep(1:3, times = n),
                  d = 2, type = "jsd", h = 0.5)
```

24 index_ridge

Description

Indexing of an unordered collection of points defining the estimated density ridge curve. The indexing is done by a multidimensional scaling map to the real line, while the smoothing is done by local polynomial regression for polyspherical-on-scalar regression.

Usage

```
index_ridge(endpoints, X, d, l_index = 1000, f_index = 2, probs_scores = seq(0, 1, l = 101), verbose = FALSE, type_bwd = c("1se", "min")[1], p = 0, ...)
```

Arguments

endpoints	a matrix of size $c(nx, sum(d) + r)$ with the end points of the ridge algorithm to be indexed.
X	a matrix of size $c(n, sum(d) + r)$ with the sample.
d	vector of size r with dimensions.
l_index	length of the grid index used for finding projections. Defaults to 1e3.
f_index	factor with the range of the grid for finding ridge projections. Defaults to 2, which is twice the range of MDS indexes.
probs_scores	probabilities for indexing the ridge on the probs_scores-quantiles of the scores. Defaults to $seq(0, 1, 1 = 101)$.
verbose	show diagnostic plots? Defaults to FALSE.
type_bwd	type of cross-validation bandwidth for Nadaraya-Watson, either "min" (minimizer of the cross-validation loss) or "1se" (the "one standard error rule", smoother). Defaults to "1se".
р	degree of local fit, either 0 or 1. Defaults to 0.
	further arguments passed to bw_cv_kre_polysph.

Details

Indexing is designed to work with collection of ridge points that admit a linear ordering, so that mapping to the real line by multidimensional scaling is adequate. The indexing will not work properly if the ridge points define a closed curve.

index_ridge 25

Value

A list with the following fields:

```
a vector of size n with the SIER scores for X.
scores_X
                  a matrix of size c(n, sum(d) + r) with the projections of X onto the SIER.
projs_X
ord_X
                  a vector of size n with the ordering of X induced by the SIER scores.
scores_grid
                  a vector of size length(probs_scores) with score quantiles associated to the
                  probabilities probs_scores.
ridge_grid
                  a vector of size length(probs_scores) with the SIER evaluated at scores_grid.
mds_index
                  a vector of size nx with the multidimensional scaling indexes.
ridge_fun
                  a function that parametrizes the SIER.
                  bandwidth used for the local polynomial regression.
probs_scores
                  object probs_scores.
```

```
## Test on (S^1)^2
# Sample
set.seed(132121)
r < -2
d \leftarrow rep(1, r)
n <- 200
ind_dj <- comp_ind_dj(d = d)</pre>
Th \leftarrow matrix(runif(n = n * (r - 1), min = -pi / 2, max = pi / 2),
              nrow = n, ncol = r - 1)
Th[, r - 1] \leftarrow sort(Th[, r - 1])
Th <- cbind(Th, sdetorus::toPiInt(</pre>
  pi + Th[, r - 1] + runif(n = n, min = -pi / 4, max = pi / 4)))
X <- angles_to_torus(Th)</pre>
col_X_alp <- viridis::viridis(n, alpha = 0.25)</pre>
col_X <- viridis::viridis(n)</pre>
# Euler
h_{rid} \leftarrow rep(0.75, r)
h_{eu} \leftarrow h_{rid^2}
N <- 200
eps <- 1e-6
Y \leftarrow euler\_ridge(x = X, X = X, d = d, h = h\_rid, h\_euler = h\_eu,
                   N = N, eps = eps, keep_paths = TRUE)
# Visualization
i <- N # Between 1 and N
plot(rbind(torus_to_angles(Y$paths[, , 1])), col = col_X_alp, pch = 19,
     axes = FALSE, xlim = c(-pi, pi), ylim = c(-pi, pi),
     xlab = "", ylab = "")
points(rbind(torus_to_angles(Y$paths[, , i])), col = col_X, pch = 16,
       cex = 0.75)
sdetorus::torusAxis(1:2)
```

26 interp_polysph

interp_polysph

Interpolation on the polysphere

Description

Creates a sequence of points on the polysphere linearly interpolating between two points extrinsically.

Usage

```
interp_polysph(x, y, ind_dj, N = 10)
```

Arguments

```
    a vector of size sum(d) + r with the begin point.
    a vector of size sum(d) + r with the end point.
    ind_dj
    0-based index separating the blocks of spheres that is computed with comp_ind_dj.
    number of points in the sequence. Defaults to 10.
```

Value

A matrix of size c(N, sum(d) + r) with the interpolation.

```
interp_polysph(x = c(1, 0), y = c(0, 1), ind_dj = comp_ind_dj(d = 1))
```

kde_polysph 27

kde_polysph	Polyspherical kernel density estimator

Description

Computes the kernel density estimator for data on the polysphere $S^{d_1} \times \cdots \times S^{d_r}$. Given a sample X_1, \dots, X_n , this estimator is

$$\hat{f}(\boldsymbol{x};\boldsymbol{h}) = \sum_{i=1}^n L_{\boldsymbol{h}}(\boldsymbol{x},\boldsymbol{X}_i)$$

for a kernel L and a vector of bandwidths h.

Usage

```
kde_polysph(x, X, d, h, weights = as.numeric(c()), log = FALSE,
  wrt_unif = FALSE, normalized = TRUE, intrinsic = FALSE,
  norm_x = FALSE, norm_X = FALSE, kernel = 1L, kernel_type = 1L,
  k = 10)
```

Arguments

X	a matrix of size $c(nx, sum(d) + r)$ with the evaluation points.
Χ	a matrix of size $c(n, sum(d) + r)$ with the sample.
d	vector of size r with dimensions.
h	vector of size r with bandwidths.
weights	weights for each observation. If provided, a vector of size n with the weights for multiplying each kernel. If not provided, set internally to rep(1 / n , n), which gives the standard estimator.
log	compute the logarithm of the density? Defaults to FALSE.
wrt_unif	flag to return a density with respect to the uniform measure. If $FALSE$ (default), the density is with respect to the Lebesgue measure.
normalized	flag to compute the normalizing constant of the kernel and include it in the kernel density estimator. Defaults to TRUE.
intrinsic	use the intrinsic distance, instead of the extrinsic-chordal distance, in the kernel? Defaults to FALSE.
norm_x, norm_X	ensure a normalization of the data? Defaults to FALSE.
kernel	kernel employed: 1 for von Mises–Fisher (default); 2 for Epanechnikov; 3 for softplus.
kernel_type	type of kernel employed: 1 for product kernel (default); 2 for spherically symmetric kernel.
k	softplus kernel parameter. Defaults to 10.0.

Value

A column vector of size c(nx, 1) with the evaluation of kernel density estimator.

28 kernel

Examples

```
# Simple check on S^1 x S^2 n < 1e3 d < c(1, 2) mu < c(0, 1, 0, 0, 1) ext{kappa} < c(5, 5) ext{h} < c(0.2, 0.2) ext{X} < r_vmf_polysph(n = n, d = d, mu = mu, kappa = kappa) ext{kde_polysph(x = rbind(mu), X = X, d = d, h = h)} ext{d} < rbind(mu), d = d, mu = mu, kappa = kappa)
```

kernel

Kernels on the hypersphere and their derivatives

Description

An isotropic kernel L on \mathcal{S}^d and its normalizing constant are such that $\int_{\mathcal{S}^d} c(h,d,L) L\left(\frac{1-x'y}{h^2}\right) \,\mathrm{d}\boldsymbol{x} = 1$ (extrinsic-chordal distance) or $\int_{\mathcal{S}^d} c(h,d,L) L\left(\frac{\cos^{-1}(x'y)^2}{2h^2}\right) \,\mathrm{d}\boldsymbol{x} = 1$ (intrinsic distance).

Usage

```
L(t, kernel = "1", squared = FALSE, deriv = 0, k = 10,
  inc_sfp = TRUE)

c_kern(h, d, kernel = "1", kernel_type = "1", k = 10, log = FALSE,
  inc_sfp = TRUE, intrinsic = FALSE)

grad_L(x, y, h, kernel = 1, k = 10)

hess_L(x, y, h, kernel = 1, k = 10)
```

Arguments

t	vector with the evaluation points.
kernel	kernel employed: 1 for von Mises–Fisher (default); 2 for Epanechnikov; 3 for softplus.
squared	square the kernel? Only for deriv = 0. Defaults to FALSE.
deriv	kernel derivative. Must be 0, 1, or 2. Defaults to 0.
k	softplus kernel parameter. Defaults to 10.0.
inc_sfp	include softplus(k) in the constant? Defaults to TRUE.
h	vector of size r with bandwidths.
d	vector of size r with dimensions.
kernel_type	type of kernel employed: 1 for product kernel (default); 2 for spherically symmetric kernel.

kre_polysph 29

```
log compute the logarithm of the constant? Defaults to FALSE.

intrinsic consider the intrinsic distance? Defaults to FALSE.

x a matrix of size c(nx, sum(d) + r) with the evaluation points.

y center of the kernel, a vector of size sum(d) + r.
```

Details

The gradient and Hessian are computed for the functions $x \mapsto L\left(\frac{1-x'y}{h^2}\right)$.

Value

- L: a vector with the kernel evaluated at t.
- grad_L: a vector with the gradient evaluated at x.
- hess_L: a matrix with the Hessian evaluated at x.

Examples

```
# Constants in terms of h
h_{grid} \leftarrow seq(0.01, 4, 1 = 100)
r <- 2
d <- 2
dr \leftarrow rep(d, r)
c_vmf <- sapply(h_grid, function(hi)</pre>
  log(c_kern(h = rep(hi, r), d = dr, kernel = 1, kernel_type = 2)))
c_epa <- sapply(h_grid, function(hi)</pre>
  log(c_kern(h = rep(hi, r), d = dr, kernel = 2, kernel_type = 2)))
c_sfp <- sapply(h_grid, function(hi)</pre>
  log(c_kern(h = rep(hi, r), d = dr, kernel = 3, k = 1, kernel_type = 2)))
plot(h_grid, c_epa, type = "l", ylab = "Constant", xlab = "h", col = 2)
lines(h_grid, c_sfp, col = 3)
lines(h_grid, c_vmf, col = 1)
abline(v = sqrt(2), lty = 2, col = 2)
# Kernel and its derivatives
h < -0.5
x <- c(sqrt(2), -sqrt(2), 0) / 2
y <- c(-sqrt(2), sqrt(3), sqrt(3)) / 3
L(t = (1 - sum(x * y)) / h^2)
grad_L(x = x, y = y, h = h)
hess_L(x = x, y = y, h = h)
```

kre_polysph

Local polynomial estimator for polyspherical-on-scalar regression

Description

Computes a local constant (Nadaraya–Watson) or local linear estimator with polyspherical response and scalar predictor.

Usage

```
kre_polysph(x, X, Y, d, h, p = 0)
```

Arguments

X	a vector of size nx with the evaluation points.
X	a vector of size n with the predictor sample.
Υ	a matrix of size $c(n, sum(d) + r)$ with the response sample on the polysphere.
d	vector of size r with dimensions.
h	a positive scalar giving the bandwidth.
р	degree of local fit, either 0 or 1. Defaults to 0.

Value

A vector of size nx with the estimated regression curve evaluated at x.

Examples

log_cv_kde_polysph

Cross-validation for the polyspherical kernel density estimator

Description

Computes the logarithm of the cross-validated kernel density estimator: $\log \hat{f}_{-i}(X_i; h)$, i = 1, ..., n.

Usage

```
log_cv_kde_polysph(X, d, h, weights = as.numeric(c()), wrt_unif = FALSE,
normalized = TRUE, intrinsic = FALSE, norm_X = FALSE, kernel = 1L,
kernel_type = 1L, k = 10)
```

Arguments

Χ	a matrix of size c(n, sum(d) + r) with the sample.
d	vector of size r with dimensions.
h	vector of size r with bandwidths.
weights	weights for each observation. If provided, a vector of size n with the weights for multiplying each kernel. If not provided, set internally to rep(1 / n , n), which gives the standard estimator.
wrt_unif	flag to return a density with respect to the uniform measure. If FALSE (default), the density is with respect to the Lebesgue measure.
normalized	flag to compute the normalizing constant of the kernel and include it in the kernel density estimator. Defaults to TRUE.
intrinsic	use the intrinsic distance, instead of the extrinsic-chordal distance, in the kernel? Defaults to FALSE.
norm_X	ensure a normalization of the data? Defaults to FALSE.
kernel	kernel employed: 1 for von Mises-Fisher (default); 2 for Epanechnikov; 3 for softplus.
kernel_type	type of kernel employed: 1 for product kernel (default); 2 for spherically symmetric kernel.
k	softplus kernel parameter. Defaults to 10.0.

Value

A column vector of size c(n, 1) with the evaluation of the logarithm of the cross-validated kernel density estimator.

Examples

```
# Simple check on S^1 x S^2
n <- 5
d <- c(1, 2)
h <- c(0.2, 0.2)
X <- r_unif_polysph(n = n, d = d)
log_cv_kde_polysph(X = X, d = d, h = h)
kde_polysph(X = X[1, , drop = FALSE], X = X[-1, ], d = d, h = h, log = TRUE)</pre>
```

Description

Computation of the polylogarithm $\text{Li}_s(-e^{\mu})$.

Usage

```
polylog_minus_exp_mu(mu, s, upper = Inf, ...)
```

Arguments

mu	vector with exponents of the negative argument.
S	vector with indexes of the polylogarithm.
upper	upper limit of integration. Defaults to Inf.
	further arguments passed to integrate, such as upper, abs.tol, rel.tol, etc.

Details

If s is an integer, 1/2, 3/2, or 5/2, then routines from the GSL library to compute Fermi–Dirac integrals are called. Otherwise, numerical integration is used.

Value

A vector of size length(mu) or length(s) with the values of the polylogarithm.

Examples

```
polylog_minus_exp_mu(mu = 1:5, s = 1)
polylog_minus_exp_mu(mu = 1, s = 1:5)
polylog_minus_exp_mu(mu = 1:5, s = 1:5)
```

proj_grad_kde_polysph Projected gradient of the polyspherical kernel density estimator

Description

Computes the projected gradient $D_{(p-1)}\hat{f}(\boldsymbol{x};\boldsymbol{h})$ of the kernel density estimator $\hat{f}(\boldsymbol{x};\boldsymbol{h})$ on the polysphere $\mathcal{S}^{d_1}\times\cdots\times\mathcal{S}^{d_r}$, where $p=\sum_{j=1}^r d_j+r$ is the dimension of the ambient space.

Usage

```
proj_grad_kde_polysph(x, X, d, h, weights = as.numeric(c()),
  wrt_unif = FALSE, normalized = TRUE, norm_x = FALSE, norm_X = FALSE,
  kernel = 1L, kernel_type = 1L, k = 10, proj_alt = TRUE,
  fix_u1 = TRUE, sparse = FALSE)
```

Arguments

X	a matrix of size $c(nx, sum(d) + r)$ with the evaluation points.
Χ	a matrix of size $c(n, sum(d) + r)$ with the sample.
d	vector of size r with dimensions.
h	vector of size r with bandwidths.
weights	weights for each observation. If provided, a vector of size n with the weights for multiplying each kernel. If not provided, set internally to rep(1 / n , n), which gives the standard estimator.

proj_polysph 33

flag to return a density with respect to the uniform measure. If FALSE (default), wrt_unif the density is with respect to the Lebesgue measure. normalized flag to compute the normalizing constant of the kernel and include it in the kernel density estimator. Defaults to TRUE. ensure a normalization of the data? Defaults to FALSE. norm_x, norm_X kernel kernel employed: 1 for von Mises-Fisher (default); 2 for Epanechnikov; 3 for softplus. kernel_type type of kernel employed: 1 for product kernel (default); 2 for spherically symmetric kernel. k softplus kernel parameter. Defaults to 10.0. proj_alt alternative projection. Defaults to TRUE. fix_u1 ensure the u_1 vector is different from x? Prevents the Euler algorithm to "surf the ridge". Defaults to TRUE. use a sparse eigendecomposition of the Hessian? Defaults to FALSE. sparse

Value

A list with the following components:

a matrix of size c(nx, sum(d) + r) with the projected gradient evaluated at x.

a matrix of size c(nx, sum(d) + r) with the first non-null Hessian eigenvector evaluated at x.

lamb_norm

a matrix of size c(nx, sum(d) + r) with the Hessian eigenvalues (largest to smallest) evaluated at x.

Examples

```
# Simple check on (S^1)^2
n <- 3
d <- c(1, 1)
mu <- c(0, 1, 0, 1)
kappa <- c(5, 5)
h <- c(0.2, 0.2)
X <- r_vmf_polysph(n = n, d = d, mu = mu, kappa = kappa)
proj_grad_kde_polysph(x = X, X = X, d = d, h = h)</pre>
```

proj_polysph

Projection onto the polysphere

Description

Projects points on $\mathbb{R}^{d_1+\cdots+d_r+r}$ onto the polysphere $\mathcal{S}^{d_1}\times\cdots\times\mathcal{S}^{d_r}$ by normalizing each block of d_j coordinates.

 r_g_{kern}

Usage

```
proj_polysph(x, ind_dj)
```

Arguments

```
x a matrix of size c(n, sum(d) + r).ind_dj 0-based index separating the blocks of spheres that is computed with comp_ind_dj.
```

Value

A matrix of size c(n, sum(d) + r) with the projected points.

Examples

```
# Example on (S^1)^2
d <- c(1, 1)
x <- rbind(c(2, 0, 1, 1))
proj_polysph(x, ind_dj = comp_ind_dj(d))</pre>
```

r_g_kern

Sample from the angular kernel density

Description

Simulation from the angular density function of an isotropic kernel on the hypersphere S^d .

Usage

```
r_g_{kern}(n, d, h, kernel = "1", k = 10)
```

Arguments

n sample size.

d vector of size r with dimensions.h vector of size r with bandwidths.

kernel employed: 1 for von Mises-Fisher (default); 2 for Epanechnikov; 3 for

softplus.

k softplus kernel parameter. Defaults to 10.0.

Value

A vector of size n with the sample.

r_kde_polysph 35

Examples

```
hist(r_g_kern(n = 1e3, d = 2, h = 1, kernel = "1"), breaks = 30,
    probability = TRUE, main = "", xlim = c(-1, 1))
hist(r_g_kern(n = 1e3, d = 2, h = 1, kernel = "2"), breaks = 30,
    probability = TRUE, main = "", xlim = c(-1, 1))
hist(r_g_kern(n = 1e3, d = 2, h = 1, kernel = "3"), breaks = 30,
    probability = TRUE, main = "", xlim = c(-1, 1))
```

r_kde_polysph

Sample from polyspherical kernel density estimator

Description

Simulates from the distribution defined by a polyspherical kernel density estimator on $\mathcal{S}^{d_1} \times \ldots \times \mathcal{S}^{d_r}$.

Usage

```
r_kde_polysph(n, X, d, h, kernel = 1, kernel_type = 1, k = 10,
norm_X = FALSE)
```

Arguments

n	sample size.
X	a matrix of size $c(n, sum(d) + r)$ with the sample.
d	vector of size r with dimensions.
h	vector of size r with bandwidths.
kernel	kernel employed: 1 for von Mises–Fisher (default); 2 for Epanechnikov; 3 for softplus.
kernel_type	type of kernel employed: 1 for product kernel (default); 2 for spherically symmetric kernel.
k	softplus kernel parameter. Defaults to 10.0.
norm_X	ensure a normalization of the data?

Details

The function uses $r_{kern_polysph}$ to sample from the considered kernel.

Value

A matrix of size c(n, sum(d) + r) with the sample.

36 r_kern_polysph

Examples

```
# Simulated data on (S^1)^2
n <- 50
samp \leftarrow r_path_s1r(n = n, r = 2, k = c(1, 2), angles = TRUE)
plot(samp, xlim = c(-pi, pi), ylim = c(-pi, pi), col = rainbow(n),
     axes = FALSE, xlab = "", ylab = "", pch = 16, cex = 0.75)
points(torus\_to\_angles(r\_kde\_polysph(n = 10 * n, X = angles\_to\_torus(samp),
                                      d = c(1, 1), h = c(0.1, 0.1)),
       col = "black", pch = 16, cex = 0.2)
sdetorus::torusAxis()
# Simulated data on S^2
n <- 50
samp <- r_path_s2r(n = n, r = 1, sigma = 0.1, kappa = 5,
                   spiral = TRUE)[, , 1]
sc3d <- scatterplot3d::scatterplot3d(</pre>
  samp, x \lim = c(-1, 1), y \lim = c(-1, 1), z \lim = c(-1, 1),
  xlab = "", ylab = "", zlab = "", color = rainbow(n), pch = 16
)
xyz \leftarrow r_kde_polysph(n = 10 * n, X = samp, d = 2, h = 0.1)
sc3d$points3d(xyz[, 1], xyz[, 2], xyz[, 3], col = "black", pch = 16,
              cex = 0.2)
```

r_kern_polysph

Sample kernel-distributed polyspherical data

Description

Simulates from the distribution defined by a kernel on the polysphere $S^{d_1} \times \cdots \times S^{d_r}$.

Usage

```
r_kern_polysph(n, d, mu, h, kernel = 1, kernel_type = 1, k = 10,
norm_mu = FALSE)
```

Arguments

n	sample size.
d	vector of size r with dimensions.
mu	a vector of size $sum(d) + r$ with the concatenated means that define the center of the kernel.
h	vector of size r with bandwidths.
kernel	kernel employed: 1 for von Mises–Fisher (default); 2 for Epanechnikov; 3 for softplus.
kernel_type	type of kernel employed: 1 for product kernel (default); 2 for spherically symmetric kernel.
k	softplus kernel parameter. Defaults to 10.0.
norm_mu	ensure a normalization of mu? Defaults to FALSE.

r_kern_polysph 37

Details

Simulation for non-von Mises–Fisher spherically symmetric kernels is done by acceptance-rejection from a von Mises–Fisher proposal distribution.

Value

A matrix of size c(n, sum(d) + r) with the sample.

```
# Simulate kernels in (S^1)^2
n <- 1e3
h < -c(1, 1)
d <- c(1, 1)
mu <- rep(DirStats::to_cir(pi), 2)</pre>
samp_ker <- function(kernel, kernel_type, col, main) {</pre>
  data <- r_kern_polysph(n = n, d = d, mu = mu, h = h, kernel = kernel,</pre>
                         kernel_type = kernel_type)
  ang <- cbind(DirStats::to_rad(data[, 1:2]),</pre>
               DirStats::to_rad(data[, 3:4]))
  plot(ang, xlim = c(0, 2 * pi), ylim = c(0, 2 * pi), pch = 16, cex = 0.25,
       col = col, xlab = expression(Theta[1]), ylab = expression(Theta[2]),
       main = main)
}
old_par <- par(mfcol = c(2, 3))
samp_ker(kernel = 2, kernel_type = 2, col = 1, main = "Epa sph. symmetric")
samp_ker(kernel = 2, kernel_type = 1, col = 2, main = "Epa product")
samp_ker(kernel = 3, kernel_type = 2, col = 1, main = "Sfp sph. symmetric")
samp_ker(kernel = 3, kernel_type = 1, col = 2, main = "Sfp product")
samp_ker(kernel = 1, kernel_type = 2, col = 1, main = "vMF sph. symmetric")
samp_ker(kernel = 1, kernel_type = 1, col = 2, main = "vMF product")
par(old_par)
# Simulate kernels in (S^2)^2
n <- 1e3
h <- c(0.2, 0.6)
d < -c(2, 2)
mu \leftarrow c(c(0, 0, 1), c(0, -1, 0))
samp_ker <- function(kernel, kernel_type, main) {</pre>
  data <- r_kern_polysph(n = n, d = d, mu = mu, h = h, kernel = kernel,
                          kernel_type = kernel_type)
  scatterplot3d::scatterplot3d(rbind(data[, 1:3], data[, 4:6]),
                                xlim = c(-1, 1), ylim = c(-1, 1),
                                zlim = c(-1, 1), pch = 16, xlab = "",
                                ylab = "", zlab = "", cex.symbols = 0.5,
       color = rep(viridis::viridis(n)[rank(data[, 3])], 2), main = main)
old_par <- par(mfcol = c(2, 3))
samp_ker(kernel = 2, kernel_type = 2, main = "Epa sph. symmetric")
samp_ker(kernel = 2, kernel_type = 1, main = "Epa product")
samp_ker(kernel = 3, kernel_type = 2, main = "Sfp sph. symmetric")
samp_ker(kernel = 3, kernel_type = 1, main = "Sfp product")
```

38 r_path_s1r

```
samp_ker(kernel = 1, kernel_type = 2, main = "vMF sph. symmetric")
samp_ker(kernel = 1, kernel_type = 1, main = "vMF product")
par(old_par)
# Plot simulated data
n <- 1e3
h < -c(1, 1)
d < -c(2, 2)
samp_ker <- function(kernel, kernel_type, col, main) {</pre>
 X <- r_kern_polysph(n = n, d = d, mu = mu, h = h, kernel = kernel,
                      kernel_type = kernel_type)
 S \leftarrow cbind((1 - X[, 1:3] %*% mu[1:3]) / h[1]^2,
             (1 - X[, 4:6] %*% mu[4:6]) / h[2]^2)
 plot(S, xlim = c(0, 2 / h[1]^2), ylim = c(0, 2 / h[2]^2), pch = 16,
       cex = 0.25, col = col, xlab = expression(t[1]),
       ylab = expression(t[2]), main = main)
 t_grid <- seq(0, 2 / min(h)^2, 1 = 100)
 gr <- as.matrix(expand.grid(t_grid, t_grid))</pre>
 if (kernel_type == "1") {
    dens <- prod(c_kern(h = h, d = d, kernel = kernel, kernel_type = 1)) *</pre>
      L(gr[, 1], kernel = kernel) * L(gr[, 2], kernel = kernel)
 } else if (kernel_type == "2") {
   dens <- c_kern(h = h, d = d, kernel = kernel, kernel_type = 2) *</pre>
      L(gr[, 1] + gr[, 2], kernel = kernel)
 dens <- matrix(dens, nrow = length(t_grid), ncol = length(t_grid))
 contour(t_grid, t_grid, dens, add = TRUE, col = col,
          levels = seq(0, 0.2, 1 = 41))
old_par <- par(mfcol = c(2, 3))
samp_ker(kernel = 2, kernel_type = 2, col = 1, main = "Epa sph. symmetric")
samp_ker(kernel = 2, kernel_type = 1, col = 2, main = "Epa product")
samp_ker(kernel = 3, kernel_type = 2, col = 1, main = "Sfp sph. symmetric")
samp_ker(kernel = 3, kernel_type = 1, col = 2, main = "Sfp product")
samp_ker(kernel = 1, kernel_type = 2, col = 1, main = "vMF sph. symmetric")
samp_ker(kernel = 1, kernel_type = 1, col = 2, main = "vMF product")
par(old_par)
```

r_path_s1r

Samplers of one-dimensional modes of variation for polyspherical data

Description

Functions for sampling data on $(\mathcal{S}^d)^r$, for d=1,2, using one-dimensional modes of variation.

r_path_s1r 39

Usage

```
r_path_s1r(n, r, alpha = runif(r, -pi, pi), k = sample(-2:2, size = r,
    replace = TRUE), sigma = 0.25, angles = FALSE)

r_path_s2r(n, r, t = 0, c = 1, Theta = t(rotasym::r_unif_sphere(n = r, p = 3)), kappa = 0, sigma = 0.25, spiral = FALSE)
```

Arguments

n	sample size.
r	number of spheres in the polysphere $(S^d)^r$.
alpha	a vector of size r valued in $[-\pi,\pi)$ with the initial angles for the linear trend. Chosen at random by default.
k	a vector of size r with the integer slopes defining the angular linear trend. Chosen at random by default.
sigma	standard deviation of the noise about the one-dimensional mode of variation. Defaults to 0.25 .
angles	return angles in $[-\pi,\pi)$? Defaults to FALSE.
t	latitude, with respect to Theta, of the small circle. Defaults to 0 (equator).
С	Clélie curve parameter, changing the spiral wrappings. Defaults to 1.
Theta	a matrix of size $c(3, r)$ giving the north poles for S^2 . Useful for rotating the sample. Chosen at random by default.
kappa	concentration von Mises–Fisher parameter for longitudes in small circles. Defaults to \emptyset (uniform).
spiral	consider a spiral (or, more precisely, a Clélie curve) instead of a small circle? Defaults to FALSE.

Value

An array of size c(n, d, r) with samples on $(S^d)^r$. If angles = TRUE for r_path_s1r, then a matrix of size c(n, r) with angles is returned.

40 r_unif_polysph

```
scatterplot3d::scatterplot3d(
  samp_2, xlim = c(-pi, pi), ylim = c(-pi, pi), zlim = c(-pi, pi),
  xlab = "", ylab = "", zlab = "", color = rainbow(n), pch = 16
# Small-circle trends on (S^2)^2
n <- 100
samp_3 \leftarrow r_path_s2r(n = n, r = 2, sigma = 0.1, kappa = 5)
old_par <- par(mfrow = c(1, 2))
scatterplot3d::scatterplot3d(
  samp_3[, , 1], xlim = c(-1, 1), ylim = c(-1, 1), zlim = c(-1, 1),
  xlab = "", ylab = "", zlab = "", color = rainbow(n), pch = 16
scatterplot3d::scatterplot3d(
  samp_3[, , 2], xlim = c(-1, 1), ylim = c(-1, 1), zlim = c(-1, 1),
  xlab = "", ylab = "", zlab = "", color = rainbow(n), pch = 16
par(old_par)
# Spiral trends on (S^2)^2
n <- 100
samp_4 \leftarrow r_path_s2r(n = n, r = 2, c = 3, spiral = TRUE, sigma = 0.01)
old_par <- par(mfrow = c(1, 2))
scatterplot3d::scatterplot3d(
  samp_4[, , 1], xlim = c(-1, 1), ylim = c(-1, 1), zlim = c(-1, 1),
  xlab = "", ylab = "", zlab = "", color = rainbow(n), pch = 16
scatterplot3d::scatterplot3d(
  samp_4[, , 2], xlim = c(-1, 1), ylim = c(-1, 1), zlim = c(-1, 1),
          ", ylab = "", zlab = "", color = rainbow(n), pch = 16
)
par(old_par)
```

r_unif_polysph

Sample uniform polyspherical data

Description

Simulates from a uniform distribution on the polysphere $S^{d_1} \times \cdots \times S^{d_r}$.

Usage

```
r_unif_polysph(n, d)
```

Arguments

```
n sample size.
```

d vector of size r with dimensions.

r_vmf_polysph 41

Value

A matrix of size c(n, sum(d) + r) with the sample.

Examples

```
# Simulate uniform data on (S^1)^2
r_unif_polysph(n = 10, d = c(1, 1))
```

r_vmf_polysph

Sample von Mises-Fisher distributed polyspherical data

Description

Simulates from a product of von Mises–Fisher distributions on the polysphere $\mathcal{S}^{d_1} \times \cdots \times \mathcal{S}^{d_r}$.

Usage

```
r_vmf_polysph(n, d, mu, kappa, norm_mu = FALSE)
```

Arguments

n sample size.

d vector of size r with dimensions.

mu a vector of size sum(d) + r with the concatenated von Mises–Fisher means.

kappa a vector of size r with the von Mises–Fisher concentrations.

norm_mu ensure a normalization of mu? Defaults to FALSE.

Value

A matrix of size c(n, sum(d) + r) with the sample.

```
# Simulate vMF data on (S^1)^2
r_vmf_polysph(n = 10, d = c(1, 1), mu = c(1, 0, 0, 1), kappa = c(1, 1))
```

view_srep

softplus

Stable computation of the softplus function

Description

Computes the softplus function $\log(1+e^t)$ in a numerically stable way for large absolute values of t

Usage

```
softplus(t)
```

Arguments

t

vector or matrix.

Value

The softplus function evaluated at t.

Examples

```
curve(softplus(10 * (1 - (1 - x) / 0.1)), from = -1, to = 1)
```

view_srep

s-rep viewer

Description

Plots a skeletal representation (s-rep) object based on its three-dimensional base, spokes, and boundary.

Usage

```
view_srep(base, dirs, bdry, radii, show_base = TRUE, show_base_pt = TRUE,
    show_bdry = TRUE, show_bdry_pt = TRUE, show_seg = TRUE,
    col_base = "red", col_bndy = "blue", col_seg = "green",
    static = TRUE, texts = NULL, cex_base = ifelse(static, 0.5, 6),
    cex_bdry = ifelse(static, 1, 8), lwd_seg = ifelse(static, 1, 2),
    cex_texts = 1, alpha_base = 0.1, alpha_bdry = 0.15, r_texts = 1.25,
    alpha_ashape3d_base = NULL, alpha_ashape3d_bdry = NULL, lit = FALSE,
    ...)
```

view_srep 43

Arguments

```
base
                  base points, a matrix of size c(nx, 3).
                  directions of spokes, a matrix of size c(nx, 3) with unit vectors.
dirs
bdry
                  boundary points, a matrix of size c(nx, 3).
radii
                  radii of spokes, a vector of size nx.
show_base, show_base_pt
                  show base and base grid? Default to TRUE.
show_bdry, show_bdry_pt
                  show boundary and boundary grid? Default to TRUE.
show_seg
                  show segments? Defaults to TRUE.
col_base, col_bndy, col_seg
                  colors for the base, boundary, and segments. Default to "red", "blue", and
                   "green", respectively.
static
                  use static (scatterplot3d) or interactive (plot3d) plot? Default to TRUE.
texts
                  add text labels? If given, it should be a vector of size nx with the labels. Defaults
                  to NULL.
cex_base, cex_bdry
                  size of the base and boundary points.
lwd_seg
                  width of the segments.
                  size of the text labels. Defaults to 1.
cex_texts
alpha_base, alpha_bdry
                  transparencies for base and boundary. Default to 0.1 and 0.15, respectively.
                  magnification of the radius to separate the text labels. Defaults to 1.25.
r_texts
alpha_ashape3d_base, alpha_ashape3d_bdry
                  alpha parameters for ashape3d. Default to NULL.
lit
                  lit parameter passed to material3d. Defaults to FALSE.
                  further arguments to be passed to plot3d or scatterplot3d.
. . .
```

Value

Creates a static or interactive plot.

Index

angles_to_polysph, 3	L (kernel), 28
angles_to_sph, 4	log_cv_kde_polysph, 30
angles_to_torus, 5	
ashape3d, <i>43</i>	material3d,43
b_d (eff_kern), 16	nlm, <i>9, 10</i>
block_euler_ridge (euler_ridge), 18	
bw_cv_kre_polysph, 6, 24	optim, 7, 8
bw_cv_polysph, 7	optimParallel, 7, 8
<pre>bw_lcv_min_epa, 8</pre>	nonellal aulan midea 11
<pre>bw_mrot_polysph, 9, 10</pre>	parallel_euler_ridge, //
bw_rot_polysph, 7, 10, 13	parallel_euler_ridge (euler_ridge), 18
	plot3d, 43 polykde (polykde-package), 3
c_kern (kernel), 28	
clean_euler_ridge, 11	polykde-package, 3
comp_ind_dj, 12, 14, 26, 34	<pre>polylog_minus_exp_mu, 31 polysph_to_angles (angles_to_polysph), 3</pre>
curv_vmf_polysph, 13	
cv.glmnet, 6	<pre>proj_grad_kde_polysph, 32 proj_polysph, 33</pre>
d_unif_polysph, 15	
d_vmf_polysph, 16	r_g_kern, 34
dist_polysph, 14	r_kde_polysph, 35
dist_polysph_cross (dist_polysph), 14	r_kern_polysph, 35, 36
<pre>dist_polysph_matrix(dist_polysph), 14</pre>	r_path_s1r, 38
	r_path_s2r (r_path_s1r), 38
eff_kern, 16	r_unif_polysph, 40
euler_ridge, <i>11</i> , 18, <i>19</i>	r_vmf_polysph,41
grad_hess_kde_polysph, 20	scatterplot3d, 43
grad_L (kernel), 28	softplus, 42
	<pre>sph_to_angles (angles_to_sph), 4</pre>
hess_L (kernel), 28	torus_to_angles (angles_to_torus), 5
hom_test_polysph, 22	torus_to_angles (angles_to_torus), 3
index_ridge, 24	v_d (eff_kern), 16
integrate, <i>17</i> , <i>32</i>	view_srep, 42
interp_polysph, 26	
kde_polysph, 27	
kernel, 28	
kre polysph. 29	