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License GPL-3

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`polykde-package` `polykde`*: Polyspherical Kernel Density Estimation*

Description

Kernel density estimation on the polysphere, (hyper)sphere, 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 (2025; doi:10.1080/01621459.2025.2521898) and García-Portugués and Meilán-Vila (2023; doi:10.1007/9783031327292_4).

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References

García-Portugués, E. and Meilán-Vila, A. (2025). Kernel density estimation with polyspherical data and its applications. *Journal of the American Statistical Association*, to appear. doi:10.1080/01621459.2025.2521898.

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

`angles_to_polysph` *Conversion between the angular and Cartesian coordinates of the polysphere*

Description

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

Usage

```
angles_to_polysph(theta, d)

polysph_to_angles(x, d)
```

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 $\mathbb{S}^{d_1} \times \cdots \times \mathbb{S}^{d_r}$. 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 (hyper)sphere*

Description

Transforms the angles $(\theta_1, \ldots, \theta_d)$ in $[0, \pi)^{d-1} \times [0, 2\pi)$ into the Cartesian coordinates

$$(\cos(x_1), \sin(x_1)\cos(x_2), \ldots, \sin(x_1) \cdots \sin(x_{d-1})\cos(x_d), \sin(x_1) \cdots \sin(x_{d-1})\sin(x_d))$$

of the sphere $\mathbb{S}^d$, 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 $\mathbb{S}^d$. Assumed to be of unit norm by rows.

Value

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

Examples

```
# Check changes of coordinates
sph_to_angles(angles_to_sph(c(pi / 2, 0, pi)))
sph_to_angles(angles_to_sph(rbind(c(pi / 2, 0, pi), c(pi, pi / 2, 4 ))))
angles_to_sph(sph_to_angles(c(0, sqrt(0.5), sqrt(0.1), sqrt(0.4))))
angles_to_sph(sph_to_angles(rbind(c(0, sqrt(0.5), sqrt(0.1), sqrt(0.4)),
                                  c(0, sqrt(0.5), sqrt(0.5), 0),
                                  c(0, 1, 0, 0),
                                  c(0, 0, 0, -1),
                                  c(0, 0, 1, 0))))
```

`angles_to_torus` *Conversion between the angular and Cartesian coordinates of the torus*

Description

Transforms the angles $(\theta_1, \ldots, \theta_d)$ in $\mathbb{T}^d = [-\pi, \pi)^d$ into the Cartesian coordinates

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

of the torus $(\mathbb{S}^1)^d$, 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 Cartesian coordinates on $(\mathbb{S}^1)^d$. 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`.

Examples

```
# 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))))
```

`bw_cv_kre_polysph` *Cross-validation bandwidth selection for polyspherical-on-scalar regression*

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

`X`	a vector of size `n` with the predictor sample.
`Y`	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, l = 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.

Examples

```
n <- 50
X <- seq(0, 1, l = 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)
```

`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,
  intrinsic = FALSE,
  type = c("LCV", "LSCV")[1],
  M = 10000,
  bw0 = NULL,
  na.rm = FALSE,
  h_min = 0,
  upscale = FALSE,
  deriv = 0,
  imp_mc = TRUE,
  seed_mc = NULL,
  exact_vmf = FALSE,
  common_h = FALSE,
  spline = FALSE,
  arcsinh = FALSE,
  opt = c("optim", "nlm")[1],
  ncores = 1,
  ...
)
```

Arguments

`X`	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.
intrinsic	use the intrinsic distance, instead of the extrinsic-chordal distance, in the kernel? Defaults to FALSE.
type	cross-validation type, either "LCV" (default) or "LSCV".
M	number of Monte Carlo samples to use for approximating the integral in the LSCV loss. Defaults to 1e4.
bw0	initial bandwidth vector for minimizing the CV loss. If NULL, it is computed internally by magnifying the bw_rot_polysph bandwidths by 50%. Can be also a matrix of initial bandwidth vectors.
na.rm	remove NAs in the objective function? Defaults to FALSE.
h_min	minimum h enforced (componentwise). Defaults to 0.
upscale	rescale the resulting bandwidths to work for derivative estimation? Defaults to FALSE.
deriv	derivative order to perform the upscaling. Defaults to 0.
imp_mc	use importance sampling in the Monte Carlo approximation of the integral in the LSCV loss? It is more accurate but also more time consuming. Defaults to TRUE.
seed_mc	seed for the Monte Carlo simulations used to estimate the integral in the LSCV loss. Defaults to NULL (no seed is fixed for different bandwidths).
exact_vmf	use the closed-form for the LSCV loss with the von Mises–Fisher kernel? Defaults to FALSE.
common_h	use the same bandwidth for all dimensions? Defaults to FALSE.
spline	use a faster spline approximation to compute Bessel functions, when available (d up to 50)?
arcsinh	do an arcsinh transformation of the LSCV loss to improve numerical stability? Defaults to FALSE.
opt	optimizer to use; either "optim" (default) or "nlm".
ncores	number of cores used during the optimization. Defaults to 1.
...	further arguments passed to optim or nlm (if ncores = 1) or optimParallel (if ncores > 1).

Details

If bw0 is a matrix, then the optimization is started at that row of bandwidths that is most promising for the optimization, i.e., the bandwidths that minimized the CV loss.

Value

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

References

García-Portugués, E. and Meilán-Vila, A. (2025). Kernel density estimation with polyspherical data and its applications. *Journal of the American Statistical Association*, to appear. doi:10.1080/01621459.2025.2521898.

Examples

```
n <- 20
d <- 1:2
kappa <- rep(10, 2)
X <- r_vmf_polysph(n = n, d = d, mu = r_unif_polysph(n = 1, d = d),
                   kappa = kappa)
bw_cv_polysph(X = X, d = d, type = "LCV")$bw
bw_cv_polysph(X = X, d = d, type = "LSCV", exact_vmf = TRUE)$bw
```

---

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: "prod" for the product kernel (default) or "sph" for the spherically symmetric kernel.

Value

The minimum bandwidth allowed.

Examples

```
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
```

`bw_mrot_polysph` *Marginal rule-of-thumb bandwidth selection for polyspherical kernel density estimator*

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

`X`	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 $\mathbb{S}^{d_1} \times \cdots \times \mathbb{S}^{d_r}$ 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`.
`kappa`	estimate of the concentration parameters. Computed if not provided (default).

Value

A vector of size `r` with the marginal optimal bandwidths.

References

García-Portugués, E. and Meilán-Vila, A. (2025). Kernel density estimation with polyspherical data and its applications. *Journal of the American Statistical Association*, to appear. doi:10.1080/01621459.2025.2521898.

Examples

```
n <- 100
d <- 1:2
kappa <- rep(10, 2)
X <- r_vmf_polysph(n = n, d = d, mu = r_unif_polysph(n = 1, d = d),
                   kappa = kappa)
bw_rot_polysph(X = X, d = d)$bw
bw_mrot_polysph(X = X, d = d)
```

`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

`X`	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: `"prod"` for the product kernel (default) or `"sph"` for the 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%. Can be also a matrix of initial bandwidth vectors.
`upscale`	rescale bandwidths to work on $\mathbb{S}^{d_1} \times \cdots \times \mathbb{S}^{d_r}$ 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 $\boldsymbol{R}$ of the unknown density is approximable by that of a product of von Mises–Fisher densities, $\boldsymbol{R}(\boldsymbol{\kappa})$. The estimation of the concentration parameters $\boldsymbol{\kappa}$ is done by maximum likelihood.

If `bw0` is a matrix, then the optimization is started at that row of bandwidths that is most promising for the optimization, i.e., the bandwidths that minimized the CV loss.

Value

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

References

García-Portugués, E. and Meilán-Vila, A. (2025). Kernel density estimation with polyspherical data and its applications. *Journal of the American Statistical Association*, to appear. doi:10.1080/01621459.2025.2521898.

Examples

```
n <- 100
d <- 1:2
kappa <- rep(10, 2)
X <- r_vmf_polysph(n = n, d = d, mu = r_unif_polysph(n = 1, d = d),
                   kappa = kappa)
bw_rot_polysph(X = X, d = d)$bw
```

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 removed. An extra logical vector removed of length nx indicates which input points were dropped.

References

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.

Examples

```
if (requireNamespace("scatterplot3d", quietly = TRUE)) {

  ## Test on S^2 with some spurious end points

  # Sample
  r <- 1
  d <- 2
  n <- 50
  ind_dj <- comp_ind_dj(d = d)
  X <- r_path_s2r(n = n, r = r, spiral = FALSE, Theta = cbind(c(1, 0, 0)),
                  sigma = 0.2)[, , 1]
  col_X <- rep(gray(0), n)
  col_X_alp <- rep(gray(0, alpha = 0.25), n)

  # Euler
  h_rid <- 0.5
```

```
h_eu <- h_rid^2
N <- 30
eps <- 1e-6
X0 <- r_unif_polysph(n = n, d = d)
Y <- 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
col_X_alp[Y_removed] <- 2

# Visualization
i <- N # Between 1 and N
sc3 <- scatterplot3d::scatterplot3d(Y$paths[, , 1], color = col_X_alp,
                                    pch = 19, xlim = c(-1, 1),
                                    ylim = c(-1, 1), zlim = c(-1, 1),
                                    xlab = "x", ylab = "y", zlab = "z")
sc3$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 = "l")

}

}
```

`comp_ind_dj` *Index of spheres on a polysphere*

Description

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

Usage

```
comp_ind_dj(d)
```

Arguments

`d`	vector of size `r` with dimensions.

Value

A vector of size `sum(d) + 1`.

Examples

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

# Example on S^1 x S^2
d <- 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 $\boldsymbol{R}(\boldsymbol{\kappa})$ 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)).

Examples

```
# Curvature matrix
d <- 2:4
kappa <- 1:3
curv_vmf_polysph(kappa = kappa, d = d)
curv_vmf_polysph(kappa = kappa, d = d, log = TRUE)

# Equivalence on the sphere with DirStats::R_Psi_mixvmf
drop(curv_vmf_polysph(kappa = kappa[1], d = d[1]))
d[1]^2 * DirStats::R_Psi_mixvmf(q = d[1], mu = rbind(c(rep(0, d[1]), 1)),
                                kappa = kappa[1], p = 1)
```

`d_mvmf_polysph` *Density of a mixture of products of von Mises–Fisher distributions on the polysphere*

Description

Computes the density of an m-mixture of product of von Mises–Fisher densities on the polysphere.

Usage

```
d_mvmf_polysph(x, d, mu, kappa, prop, log = FALSE)
```

Arguments

`x`	a matrix of size `c(nx, sum(d) + r)` with the evaluation points.
`d`	vector of size `r` with dimensions.
`mu`	a matrix of size `c(m, sum(d + 1))` with the means of each mixture components in the rows.
`kappa`	a matrix of size `c(m, r)` with the concentrations of each mixture components in the rows.
`prop`	a vector of size `m` with the proportions of the mixture components.
`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 <- c(1, 2)
mu <- rbind(c(0, 1, 0, 1, 0), c(1, 0, 1, 0, 0))
kappa <- rbind(c(5, 2), c(1, 2))
prop <- c(0.7, 0.3)
x <- r_mvmf_polysph(n = 1e4, d = d, mu = mu, kappa = kappa, prop = prop)
mean(1 / d_mvmf_polysph(x = x, d = d, mu = mu, kappa = kappa, prop = prop)) /
  prod(rotasym::w_p(p = d + 1))
```

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.

Examples

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

d_vmf_polysph *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

x	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 <- c(1, 2)
mu <- c(0, 1, 0, 1, 0)
kappa <- c(1, 1)
x <- 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))
```

---

dist_polysph *Polyspherical distance*

Description

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

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

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

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.
std	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.

Examples

```
# 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)
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)
```

`eff_kern` *Polyspherical kernel moments and efficiencies*

Description

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

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 sphere $\mathbb{S}^d$.
`r`	a scalar with the number of polyspheres of the same dimension.
`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 employed: "prod" for the product kernel (default) or "sph" for the 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. Uses the same codification as kernel_type. Defaults to "sph".
...	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 sphere (common if kernel_type = "sph").
- v_d: a vector with the second kernel moment if kernel_type = "prod", or a scalar if kernel_type = "sph".
- eff_kern: a scalar with the kernel efficiency.

See Also

kde_polysph, bw_rot_polysph.

Examples

```
# 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")
```

---

euler_ridge *Euler algorithms for polyspherical density ridge estimation*

Description

Functions to perform density ridge estimation on the polysphere $\mathbb{S}^{d_1} \times \cdots \times \mathbb{S}^{d_r}$ 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

x	a matrix of size c(nx, sum(d) + r) with the starting points for the Euler algorithm.
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.
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.
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 spheres, 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 defining 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 matrix 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 algorithm.
`iter`	a column matrix of size `c(nx, 1)` counting the iterations required for each point.
`conv`	a column matrix of size `c(nx, 1)` with convergence flags.
`d`	vector `d`.
`h`	bandwidth used for the kernel density estimator.
`error`	a column matrix of size `c(nx, 1)` indicating if errors were found for each path.

References

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

`clean_euler_ridge`, `index_ridge`, `proj_grad_kde_polysph`, `grad_hess_kde_polysph`.

Examples

```
if (requireNamespace("scatterplot3d", quietly = TRUE) &&
    requireNamespace("viridis", quietly = TRUE)) {

  ## Test on S^2 with a small circle trend

  # Sample
  r <- 1
  d <- 2
  n <- 50
  ind_dj <- 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)
  col_X <- viridis::viridis(n)

  # Euler
  h_rid <- 0.5
  h_eu <- h_rid^2
  N <- 30
  eps <- 1e-6
  Y <- euler_ridge(x = X, X = X, d = d, h = h_rid, h_euler = h_eu,
                   N = N, eps = eps, keep_paths = TRUE)
  Y

  # Visualization
  i <- N # Between 1 and N
  sc3 <- scatterplot3d::scatterplot3d(Y$paths[, , 1], color = col_X_alp,
                                      pch = 19, xlim = c(-1, 1),
                                      ylim = c(-1, 1), zlim = c(-1, 1),
                                      xlab = "x", ylab = "y", zlab = "z")
  sc3$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 = "l")

  }

}

## Parallel and block variants on (S^2)^4
set.seed(987204452)
r <- 4
d <- rep(2, r)
ind_dj <- comp_ind_dj(d = d)
n <- 30
X <- r_unif_polysph(n = n, d = d)
h_rid <- rep(0.7, r)
h_eu <- h_rid^2
# Parallel: same algorithm as euler_ridge but distributing starting points
Y_par <- parallel_euler_ridge(x = X[1:5, , drop = FALSE], X = X, d = d,
                              h = h_rid, h_euler = h_eu, N = 20, cores = 1)
# Block: marginal Euler over groups of spheres (all d's must be equal)
Y_block <- block_euler_ridge(x = X[1:5, , drop = FALSE], X = X, d = d,
                             h = h_rid, h_euler = h_eu,
                             ind_blocks = c(1, 1, 2, 2), N = 20)
```

---

fib_latt *Fibonacci lattice on the sphere*

Description

Computes the Fibonacci lattice on the sphere $\mathbb{S}^2$ to produce pseudo-equispaced points.

Usage

```
fib_latt(n)
```

Arguments

n	number of points to be produced.

Value

A matrix of size `c(n, 3)` with the spherical coordinates.

Examples

```
scatterplot3d::scatterplot3d(
  fib_latt(n = 200), pch = 19, color = viridis::viridis(200),
  xlim = c(-1, 1), ylim = c(-1, 1), zlim = c(-1, 1),
  xlab = "", ylab = "", zlab = "")
```

---

grad_hess_kde_polysph *Gradient and Hessian of the polyspherical kernel density estimator*

Description

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

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.
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.
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 fields:

dens	a column matrix of size c(nx, 1) with the kernel density estimator evaluated at x.
grad	a matrix of size c(nx, sum(d) + r) with the gradient of the kernel density estimator 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.

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)
grh <- grad_hess_kde_polysph(x = X, X = X, d = d, h = h)
str(grh)
grh
```

`hammer_to_sph` *Map Cartesian coordinates into Hammer projection*

Description

Computes the Hammer projection of points on the sphere.

Usage

```
sph_to_hammer(x)

hammer_to_sph(y)
```

Arguments

`x`	matrix of size `c(n, 3)` with the Cartesian coordinates on $\mathbb{S}^2$. Assumed to be of unit norm in the rows.
`y`	matrix of size `c(n, 2)` with the Hammer coordinates.

Value

- `sph_to_hammer`: the matrix `y`.
- `hammer_to_sph`: the matrix `x`.

Examples

```
# Plot Fibonacci lattice
plot(sph_to_hammer(fib_latt(n = 1000)))
points(sph_to_hammer(rbind(c(0, 0, 1), c(0, 0, -1))), col = 2, pch = 19)
points(sph_to_hammer(rbind(c(1, 0, 0), c(-1, 0, 0))), col = 3, pch = 19)
points(sph_to_hammer(rbind(c(0, 1, 0), c(0, -1, 0))), col = 4, pch = 19)

# Check changes of coordinates
hammer_to_sph(sph_to_hammer(rbind(c(1, 0, 0), c(0, 1, 0))))
sph_to_hammer(hammer_to_sph(rbind(c(0, 0), c(0.5, 0.5))))
```

`hippocampus` *Skeletal representation of hippocampus shapes*

Description

Contains skeletal representations (s-reps) for the hippocampus shapes of 177 6-month-old infants. The s-reps models include 168 spokes, and hence the directions of the spokes form a sample on the polysphere $(\mathbb{S}^2)^{168}$. There are 34 infants that later developed autism.

Usage

```
hippocampus
```

Format

A list with six fields:

base an array of size `c(177, 168, 3)` with the coordinates of the base points.

bdry an array of size `c(177, 168, 3)` with the coordinates of the boundary points.

dirs an array of size `c(177, 168, 3)` with the directions of spokes (unit vectors).

rads a matrix of size `c(177, 168)` with the radii of the spokes.

ids hippocampi identifiers.

ids_labs class labels. `TRUE` stands for infants that developed autism and `FALSE` for those that did not.

Source

The fitted s-reps data was shared by Prof. Stephen M. Pizer and Dr. Zhiyuan Liu, see Liu et al. (2021) and the repository https://github.com/ZhiyLiu/shanapy. The source for the raw hippocampi data is the Infant Brain Imaging Study (IBIS) network.

References

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.

Liu, Z., Hong, J., Vicory, J., Damon, J. N. and Pizer, S. M. (2021). Fitting unbranching skeletal structures to objects. *Medical Image Analysis*, 70:102020. doi:10.1016/j.media.2021.102020

Examples

```
if (requireNamespace("scatterplot3d", quietly = TRUE)) {
  # Load data
  data("hippocampus")
  attach(hippocampus)
```

```
  # View ith hippocampus s-rep
  i <- 50
  view_srep(base = base[i, , ], dirs = dirs[i, , ], bdry = bdry[i, , ])
}
```

`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 $\mathbb{S}^{d_1} \times \cdots \times \mathbb{S}^{d_r}$. 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

`X`	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.
B	number of permutations to use. Defaults to 1e3.
M	number of Monte Carlo samples 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 in the original and bootstrapped statistics. Defaults to NULL (no seed is fixed).
cv_jsd	use cross-validation to approximate the Jensen–Shannon distance? Does not require Monte Carlo. Defaults to TRUE.

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.
n	a table with the sample sizes per group.
h	bandwidths used.
B	number of permutations.
alternative	a character string describing the alternative hypothesis.
method	the kind of test performed.
data.name	a character string giving the name of the data.

References

García-Portugués, E. and Meilán-Vila, A. (2025). Kernel density estimation with polyspherical data and its applications. *Journal of the American Statistical Association*, to appear. doi:10.1080/01621459.2025.2521898.

See Also

kde_polysph, bw_rot_polysph, bw_cv_polysph.

Examples

```
## Two-sample case

# H0 holds
n <- c(50, 100)
X1 <- rotasym::r_vMF(n = n[1], mu = c(0, 0, 1), kappa = 1)
X2 <- 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 <- 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 <- rotasym::r_vMF(n = n[1], mu = c(0, 0, 1), kappa = 1)
X2 <- rotasym::r_vMF(n = n[2], mu = c(0, 0, 1), kappa = 1)
X3 <- 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)

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

---

index_ridge *Index a ridge curve, creating the Smoothed and Indexed Estimated Ridge (SIER)*

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, l = 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".
p	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.

Value

A list with the following fields:

scores_X	a vector of size n with the SIER scores for X.
projs_X	a matrix of size c(n, sum(d) + r) with the projections of X onto the SIER.
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.
h	bandwidth used for the local polynomial regression.
probs_scores	object probs_scores.

References

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.

Examples

```
if (requireNamespace("sdetorus", quietly = TRUE) &&
    requireNamespace("viridis", quietly = TRUE)) {

  ## Test on (S^1)^2

  # Sample
  r <- 2
  d <- rep(1, r)
  n <- 200
  ind_dj <- comp_ind_dj(d = d)
  Th <- matrix(runif(n = n * (r - 1), min = -pi / 2, max = pi / 2),
               nrow = n, ncol = r - 1)
  Th[, r - 1] <- sort(Th[, r - 1])
  Th <- cbind(Th, sdetorus::toPiInt(
    pi + Th[, r - 1] + runif(n = n, min = -pi / 4, max = pi / 4)))
  X <- angles_to_torus(Th)
  col_X_alp <- viridis::viridis(n, alpha = 0.25)
  col_X <- viridis::viridis(n)

  # Euler
  h_rid <- rep(0.75, r)
  h_eu <- h_rid^2
  N <- 200
  eps <- 1e-6
  Y <- 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)
  for (k in seq_len(nrow(Y$paths))) {

    xy <- torus_to_angles(t(Y$paths[k, , ]))
```

```
  sdetorus::linesTorus(x = xy[, 1], y = xy[, 2], col = col_X_alp[k])

}

# SIER
ind_rid <- index_ridge(endpoints = Y$ridge_y, X = X, d = d,
                       probs_scores = seq(0, 1, l = 50))
xy <- torus_to_angles(ind_rid$ridge_grid)
sdetorus::linesTorus(x = xy[, 1], y = xy[, 2], col = 2, lwd = 2)
points(torus_to_angles(ind_rid$ridge_fun(quantile(ind_rid$scores_grid))),
       col = 4, pch = 19)

# Scores
plot(density(ind_rid$scores_X), type = "l", xlab = "Scores",
     ylab = "Density", main = "Scores density")
for (i in 1:n) rug(ind_rid$scores_X[i], col = col_X[i])

}
```

`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

`x`	a vector of size `sum(d) + r` with the begin point.
`y`	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`.
`N`	number of points in the sequence. Defaults to `10`.

Value

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

Examples

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

kde_polysph *Polyspherical kernel density estimator*

Description

Computes the kernel density estimator for data on the polysphere $\mathbb{S}^{d_1} \times \cdots \times \mathbb{S}^{d_r}$. Given a sample $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n$, 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 $\boldsymbol{h}$.

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.
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.
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 matrix of size `c(nx, 1)` with the evaluation of the kernel density estimator.

References

García-Portugués, E. and Meilán-Vila, A. (2025). Kernel density estimation with polyspherical data and its applications. *Journal of the American Statistical Association*, to appear. doi:10.1080/01621459.2025.2521898.

See Also

`log_cv_kde_polysph`, `grad_hess_kde_polysph`, `r_kde_polysph`, `bw_rot_polysph`, `bw_cv_polysph`, `bw_mrot_polysph`.

Examples

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

`kernel` *Kernels on the sphere and their derivatives*

Description

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

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 <- seq(0.01, 4, l = 100)
r <- 2
d <- 2
dr <- rep(d, r)
c_vmf <- sapply(h_grid, function(hi)
  log(c_kern(h = rep(hi, r), d = dr, kernel = 1, kernel_type = 2)))
c_epa <- sapply(h_grid, function(hi)
  log(c_kern(h = rep(hi, r), d = dr, kernel = 2, kernel_type = 2)))
c_sfp <- sapply(h_grid, function(hi)
  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.
`Y`	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.
`p`	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

```
if (requireNamespace("scatterplot3d", quietly = TRUE)) {
  x_grid <- seq(-0.25, 1.25, l = 200)
  n <- 50
  X <- seq(0, 1, l = n)
  Y <- r_path_s2r(n = n, r = 1, sigma = 0.1, spiral = TRUE)[, , 1]
  h0 <- bw_cv_kre_polysph(X = X, Y = Y, d = 2, p = 0, plot_cv = FALSE)$h_1se
  sc3 <- scatterplot3d::scatterplot3d(Y, pch = 16, xlim = c(-1, 1),
                                      ylim = c(-1, 1), zlim = c(-1, 1),
                                      xlab = "", ylab = "", zlab = "")
  sc3$points3d(kre_polysph(x = x_grid, X = X, Y = Y, d = 2, h = h0, p = 0),
               pch = 16, type = "l", col = 2, lwd = 2)
  sc3$points3d(kre_polysph(x = x_grid, X = X, Y = Y, d = 2, h = h0, p = 1),
               pch = 16, type = "l", col = 3, lwd = 2)
}
```

---

log_cv_kde_polysph *Cross-validation for the polyspherical kernel density estimator*

Description

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

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

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.
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 matrix 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)
```

---

polylog_minus_exp_mu *Polylogarithm function with negative argument*

Description

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

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 $\mathsf{D}_{(p-1)}\hat{f}(\boldsymbol{x};\boldsymbol{h})$ of the kernel density estimator $\hat{f}(\boldsymbol{x};\boldsymbol{h})$ on the polysphere $\mathbb{S}^{d_1}\times\cdots\times\mathbb{S}^{d_r}$, 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.
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.
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.
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.
sparse	use a sparse eigendecomposition of the Hessian? Defaults to FALSE.

Value

A list with the following components:

eta	a matrix of size c(nx, sum(d) + r) with the projected gradient evaluated at x.
u1	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)
```

proj_polysph *Projection onto the polysphere*

Description

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

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

```
# Project an arbitrary point in R^2 x R^2 onto (S^1)^2
d <- c(1, 1)
x <- rbind(c(2, 0, 1, 1))
proj_polysph(x, ind_dj = comp_ind_dj(d))
```

r_g_kern *Sample from the angular kernel density*

Description

Simulation from the angular density function of an isotropic kernel on the sphere $\mathbb{S}^d$.

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	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.

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 $\mathbb{S}^{d_1} \times \ldots \times \mathbb{S}^{d_r}$.

Usage

```
r_kde_polysph(
  n,
  X,
  d,
  h,
  kernel = 1,
  kernel_type = 1,
  k = 10,
  intrinsic = FALSE,
  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.

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?

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.

Examples

```
if (requireNamespace("sdetorus", quietly = TRUE)) {
  # Simulated data on (S^1)^2
  n <- 50
  samp <- 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()
}

if (requireNamespace("scatterplot3d", quietly = TRUE)) {
  # 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(
    samp, xlim = c(-1, 1), ylim = c(-1, 1), zlim = c(-1, 1),
    xlab = "", ylab = "", zlab = "", color = rainbow(n), pch = 16
  )
  xyz <- 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 $\mathbb{S}^{d_1} \times \cdots \times \mathbb{S}^{d_r}$.

Usage

```
r_kern_polysph(
  n,
  d,
  mu,
  h,
  kernel = 1,
  kernel_type = 1,
  k = 10,
  intrinsic = FALSE,
  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.
intrinsic	use the intrinsic distance, instead of the extrinsic-chordal distance, in the kernel? Defaults to FALSE.
norm_mu	ensure a normalization of mu? Defaults to FALSE.

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.

Examples

```
if (requireNamespace("DirStats", quietly = TRUE)) {
  # Simulate kernels in (S^1)^2
  n <- 1e3
  h <- c(1, 1)
  d <- c(1, 1)
  mu <- rep(DirStats::to_cir(pi), 2)
  samp_ker <- function(kernel, kernel_type, col, main) {
```

```
    data <- r_kern_polysph(n = n, d = d, mu = mu, h = h, kernel = kernel,
                           kernel_type = kernel_type)
    ang <- cbind(DirStats::to_rad(data[, 1:2]),
                 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)
}

if (requireNamespace("scatterplot3d", quietly = TRUE) &&
    requireNamespace("viridis", quietly = TRUE)) {

  # Simulate kernels in (S^2)^2
  n <- 1e3
  h <- c(0.2, 0.6)
  d <- c(2, 2)
  mu <- c(c(0, 0, 1), c(0, -1, 0))
  samp_ker <- function(kernel, kernel_type, main) {
    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")
  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) {
  X <- r_kern_polysph(n = n, d = d, mu = mu, h = h, kernel = kernel,
                      kernel_type = kernel_type)
  S <- 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, l = 100)
  gr <- as.matrix(expand.grid(t_grid, t_grid))
  if (kernel_type == "1") {

    dens <- prod(c_kern(h = h, d = d, kernel = kernel, kernel_type = 1)) *
      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) *
      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, l = 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_mvmf_polysph` *Sample mixtures of von Mises–Fisher distributed polyspherical data*

Description

Simulates from an m-mixture of product of von Mises–Fisher distributions on the polysphere $\mathbb{S}^{d_1} \times \cdots \times \mathbb{S}^{d_r}$.

Usage

```
r_mvmf_polysph(n, d, mu, kappa, prop, norm_mu = FALSE)
```

Arguments

`n`	sample size.
`d`	vector of size `r` with dimensions.

mu	a matrix of size c(m, sum(d + 1)) with the means of each mixture components in the rows.
kappa	a matrix of size c(m, r) with the concentrations of each mixture components in the rows.
prop	a vector of size m with the proportions of the mixture components.
norm_mu	ensure a normalization of mu? Defaults to FALSE.

Value

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

Examples

```
# Simulate mixture of vMF data on (S^1)^2
r_mvmf_polysph(n = 10, d = c(1, 1),
               mu = rbind(c(0, 1, 0, 1), c(1, 0, 1, 0)),
               kappa = rbind(c(5, 2), c(1, 2)), prop = c(0.7, 0.3))
```

---

r_path_s1r *Samplers of one-dimensional modes of variation for polyspherical data*

Description

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

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 $(\mathbb{S}^d)^r$.
alpha	a vector of size r valued in $\mathbb{T} = [-\pi, \pi)$ 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 $\mathbb{T} = [-\pi, \pi)$? Defaults to FALSE.
t	latitude, with respect to Theta, of the small circle. Defaults to 0 (equator).
c	Clélie curve parameter, changing the spiral wrappings. Defaults to 1.
Theta	a matrix of size c(3, r) giving the north poles for $\mathbb{S}^2$. Useful for rotating the sample. Chosen at random by default.
kappa	concentration von Mises–Fisher parameter for longitudes in small circles. Defaults to 0 (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 $(\mathbb{S}^d)^r$. If angles = TRUE for r_path_s1r, then a matrix of size c(n ,r) with angles is returned.

See Also

r_unif_polysph, r_vmf_polysph, r_mvmf_polysph, r_kern_polysph, r_kde_polysph.

Examples

```
if (requireNamespace("sdetorus", quietly = TRUE)) {
  # Straight trends on (S^1)^2
  n <- 100
  samp_1 <- r_path_s1r(n = n, r = 2, k = c(1, 2), angles = TRUE)
  plot(samp_1, xlim = c(-pi, pi), ylim = c(-pi, pi), col = rainbow(n),
       axes = FALSE, xlab = "", ylab = "", pch = 16)
  sdetorus::torusAxis()
}


if (requireNamespace("sdetorus", quietly = TRUE) &&
    requireNamespace("scatterplot3d", quietly = TRUE)) {

  # Straight trends on (S^1)^3
  n <- 100
  samp_2 <- r_path_s1r(n = n, r = 3, angles = TRUE)
  pairs(samp_2, xlim = c(-pi, pi), ylim = c(-pi, pi), col = rainbow(n),
```

```
      pch = 16)
  sdetorus::torusAxis()
  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 <- 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 <- 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),
    xlab = "", 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 $\mathbb{S}^{d_1} \times \cdots \times \mathbb{S}^{d_r}$.

Usage

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

Arguments

n	sample size.
d	vector of size r with dimensions.

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 $\mathbb{S}^{d_1} \times \cdots \times \mathbb{S}^{d_r}$.

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.

Examples

```
# 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))
```

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,
  ...
)
```

Arguments

base	base points, a matrix of size c(nx, 3).
dirs	directions of spokes, a matrix of size c(nx, 3) with unit vectors.
bdry	boundary points, a matrix of size c(nx, 3). Optional; computed internally as base + radii * dirs if missing.
radii	radii of spokes, a vector of size nx. Optional; computed internally from base and bdry if missing.
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.
cex_texts	size of the text labels. Defaults to 1.
alpha_base, alpha_bdry	transparencies for base and boundary. Default to 0.1 and 0.15, respectively.
r_texts	magnification of the radius to separate the text labels. Defaults to 1.25.
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

Invisibly returns `NULL`. Called for the side effect of producing a static or interactive 3D plot of the s-rep.

References

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

`hippocampus`, `interp_polysph`.

Examples

```
if (requireNamespace("scatterplot3d", quietly = TRUE)) {
  base <- r_unif_polysph(n = 50, d = 2)
  dirs <- base
  radii <- runif(nrow(base), min = 0.5, max = 1)
  bdry <- base + radii * dirs
  view_srep(base = base, dirs = dirs, bdry = bdry, radii = radii,
            texts = 1:50, xlim = c(-2, 2), ylim = c(-2, 2), zlim = c(-2, 2))
}
```

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