Package: geosmooth (via r-universe)

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Title Geometric Smoothing and Conditional Expectation Methods

Version 0.1.0

Description Provides geometric methods for nonparametric regression and density estimation on data represented as coordinate matrices or weighted graphs. Methods include local polynomial smoothing, model-averaged local polynomial smoothing, local polynomial lifting trend filtering, synchronized local polynomial lifting trend filtering, graph low-pass filtering, and Hessian-energy regression. Methodological references include Gajer and Ravel (2025) ``Adaptive Geometric Regression for High-Dimensional Structured Data'' <doi:10.48550/arXiv.2511.03817>, Fan and Gijbels (1996, ISBN:9780412983214), Wang et al. (2016) ``Trend Filtering on Graphs'' <https://www.jmlr.org/papers/v17/15-147.html>, and Kim et al. (2009) ``Semi-Supervised Regression Using Hessian Energy'' <https://papers.nips.cc/paper/3741-semi-supervised-regression-using-hessian-energy-with-an-application-to-semi-supervised-dimer

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BugReports https://github.com/pgajer/geosmooth/issues

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`geosmooth-package` *geosmooth package*

Description

Geometric smoothing and conditional expectation methods for coordinate data, point clouds, and weighted graphs. The package provides local polynomial, model-averaged, trend-filtering, graph low-pass, occupation-density, and Hessian-energy methods.

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See Also

Useful links:

- https://github.com/pgajer/geosmooth
- Report bugs at https://github.com/pgajer/geosmooth/issues

`apply.metric.graph.lowpass.path` *Apply a Metric Graph Low-Pass Filter Path*

Description

Applies every requested low-pass parameter to one response or a matrix of responses using a reusable spectral basis.

Usage

```
apply.metric.graph.lowpass.path(
  basis,
  y,
  eta.grid,
  filter.type = c("heat_kernel", "tikhonov", "cubic_spline", "gaussian", "exponential",
    "butterworth"),
  block.size = NULL,
  truncation.tol = 1e-04,
  unresolved.action = c("warn", "error", "allow"),
  exact.zero = TRUE
)
```

Arguments

basis	A "metric.graph.lowpass.basis" object.
y	Numeric response vector or matrix with one row per graph vertex.
eta.grid	Numeric filter-parameter grid.
filter.type	Spectral low-pass filter family.
block.size	Optional number of response columns processed together.
truncation.tol	Positive tolerance smaller than one used to classify truncated-basis candidates as spectrally resolved.
unresolved.action	Action when a truncated-basis candidate exceeds truncation.tol: "warn", "error", or "allow".
exact.zero	Logical. For heat filtering, return the input exactly at eta = 0. This avoids treating a truncated spectral projection as the identity.

Value

A list of class "metric.graph.lowpass.path". For one response, fitted.values is an N by J matrix. For multiple responses it is an N by J by S array.

Examples

```
adj <- list(2L, c(1L, 3L), c(2L, 4L), 3L)
lengths <- list(1, c(1, 1), c(1, 1), 1)
basis <- metric.graph.lowpass.basis(adj, lengths, n.eigenpairs = 4L,
                                    eigen.solver = "dense")
apply.metric.graph.lowpass.path(basis, 1:4, eta.grid = c(0, 0.1, 1))
```

---

as.data.frame.synthetic_dataset

Summarize a synthetic dataset as one metadata row

Description

Summarize a synthetic dataset as one metadata row

Usage

```
## S3 method for class 'synthetic_dataset'
as.data.frame(x, row.names = NULL, optional = FALSE, ...)
```

Arguments

x	A synthetic_dataset.
row.names	Optional row names.
optional	Ignored.
...	Ignored.

Value

A one-row data frame.

`bootstrap.malps` *Bootstrap Uncertainty For A Fixed-Selection MALPS Fit*

Description

Reuses the supports, local charts, prediction supports, averaging weights, selected degree, and local-solver controls from an existing `fit.malps` object, then repeatedly calls `refit.malps` with bootstrap-style case weights. This is a fixed-selection uncertainty diagnostic: it measures refit variability conditional on the fitted MALPS support profile and does not rerun cross-validation or rebuild supports in each replicate.

Usage

```
bootstrap.malps(
  object,
  B = 200L,
  weight.type = c("bayesian", "multinomial"),
  y = NULL,
  probs = NULL,
  conf.level = 0.95,
  seed = NULL,
  max.failures = max(10L, B),
  keep.weights = FALSE,
  verbose = FALSE,
  ...
)
```

Arguments

`object`	A `"malps"` object from `fit.malps` or `refit.malps`.
`B`	Number of successful bootstrap replicates requested.
`weight.type`	Bootstrap weight generator, one of `"bayesian"` or `"multinomial"`.
`y`	Optional response vector. Defaults to `object$y`.
`probs`	Optional nonnegative sampling probabilities for `weight.type = "multinomial"`.
`conf.level`	Pointwise interval level used in the returned summary.
`seed`	Optional integer seed for reproducible bootstrap weights.
`max.failures`	Maximum failed refit attempts allowed before stopping.
`keep.weights`	Logical; store the generated bootstrap weights in the returned object.
`verbose`	Logical; emit progress messages every ten successful replicates.
`...`	Reserved for future extensions.

Details

Two weight generators are available. `"bayesian"` draws positive exponential weights and rescales them to have mean one. This is the default because it preserves positive local support weights and therefore avoids many local-support degeneracies. `"multinomial"` draws ordinary nonparametric bootstrap counts with total count `nrow(object$X)`; this can fail when a replicate assigns zero weight to all observations in a local support, and such failures are recorded.

Value

A list of class `"malps_bootstrap"` containing:

- `replicate.fitted.values`: an $n \times B$ matrix of successful replicate fitted values;
- `replicate.weights`: an optional $n \times B$ matrix of bootstrap weights when `keep.weights = TRUE`;
- `failures`: a data frame with columns `attempt`, `failure`, and `message`;
- `summary`: pointwise fitted values, bootstrap summaries, and empirical lower/upper intervals;
- bootstrap metadata such as `B.completed`, `n.failures`, `conf.level`, and `weight.type`.

Examples

```
X <- matrix(seq(0, 1, length.out = 20), ncol = 1)
fit <- fit.malps(X, X[, 1]^2, degree = 1L,
                 support.type = "knn", support.size = 8L)
bootstrap.malps(fit, B = 5L, seed = 1L)
```

`compare.synthetic.dataset` *Compare two synthetic datasets scientifically*

Description

Compare two synthetic datasets scientifically

Usage

```
compare.synthetic.dataset(x, y, tolerance = c(1e-12, 1e-10))
```

Arguments

`x, y`	Synthetic datasets.
`tolerance`	Absolute-plus-relative comparison tolerance.

Value

A list with equality and mismatch details.

Examples

```
spec <- synthetic.registry.spec("G1")
x <- materialize.synthetic(spec, n = 20L, seed = 1L)
y <- materialize.synthetic(spec, n = 20L, seed = 1L)
compare.synthetic.dataset(x, y)
```

---

edge.lengths.synthetic.geometry

Exact latent-segment lengths under a synthetic geometry

Description

For quadforms this integrates the induced metric along each straight latent segment. Flat quadforms reduce exactly to Euclidean distance.

Usage

```
edge.lengths.synthetic.geometry(geometry, from, to, tolerance = 1e-10)
```

Arguments

geometry	A synthetic_quadform_geometry.
from, to	Matching endpoint matrices with one segment per row.
tolerance	Positive integration tolerance.

Value

A numeric vector of segment lengths.

Examples

```
geometry <- synthetic.quadform(1L, 1L)
edge.lengths.synthetic.geometry(geometry, matrix(0), matrix(2))
```

---

embed.synthetic.geometry

Embed latent coordinates through a synthetic geometry

Description

This deterministic operator performs no random draws. A realized frame.matrix is required for random-frame geometries.

Usage

```
embed.synthetic.geometry(geometry, latent, frame.matrix = NULL)
```

Arguments

geometry	A synthetic geometry component.
latent	Latent coordinates in rows.
frame.matrix	Optional realized orthonormal frame.

Value

A numeric matrix of observed coordinates.

Examples

```
geometry <- synthetic.circle()
embed.synthetic.geometry(geometry, matrix(c(0, pi / 2), ncol = 1))
```

---

fit.chart.kernel *Fit a Chart-Kernel Smoother*

Description

Fits a local chart-kernel field by evaluating a Nadaraya–Watson style smoother at each evaluation point. The function is a general fitted-field model, not an occupation-density wrapper: density workflows should call normalize.density on the returned fit.

Usage

```
fit.chart.kernel(
  X,
  y,
  X.eval = NULL,
  support.size = min(15L, nrow(X)),
  kernel = c("gaussian", "tricube", "epanechnikov", "triangular"),
  bandwidth.multiplier = 1,
  support.grid = NULL,
  kernel.grid = NULL,
  bandwidth.multiplier.grid = NULL,
  foldid = NULL,
  cv.folds = 5L,
  cv.seed = 1L,
  coordinate.method = c("coordinates", "local.pca"),
  chart.dim = NULL,
  chart.dim.grid = NULL,
  selection.strategy = c("grid", "sparse_kd", "plateau_kd"),
  chart.dim.max = NULL,
  geometry.margin = 0L,
  auto.chart.support.metric = c("coordinates", "operator", "both"),
  auto.chart.selection.metric = c("coordinates", "operator"),
```

```
  quadrature.weights = NULL,
  denominator.floor = sqrt(.Machine$double.eps),
  return.details = TRUE
)
```

Arguments

X	Numeric matrix with one row per source/support point.
y	Numeric response or mass vector of length nrow(X).
X.eval	Optional numeric matrix of evaluation points. Defaults to X.
support.size	Number of source points in each local support.
kernel	Kernel name. Supported values are "gaussian", "tricube", "epanechnikov", and "triangular".
bandwidth.multiplier	Positive multiplier applied to the local support radius.
support.grid	Optional integer candidate neighborhood sizes. If supplied, or if foldid is supplied, the function performs row-wise cross-validation and refits the selected candidate on all rows.
kernel.grid	Optional kernel candidates for cross-validation.
bandwidth.multiplier.grid	Optional bandwidth-multiplier candidates for cross-validation.
foldid	Optional positive integer vector assigning source rows to cross-validation folds.
cv.folds	Number of folds used when foldid is not supplied.
cv.seed	Random seed used to generate folds when foldid is not supplied.
coordinate.method	Local coordinate method. "coordinates" uses centered ambient coordinates. "local.pca" projects centered support points onto a local PCA basis.
chart.dim	Local PCA dimension when coordinate.method = "local.pca". If NULL, the dimension is min(ncol(X), support.size - 1). The deployable input-only policies "auto" and "local.auto" use the same local-PCA dimension diagnostics as fit.lps; "auto" resolves one global chart dimension, while "local.auto" resolves one dimension per evaluation anchor.
chart.dim.grid	Optional candidate chart dimensions for experimental row-wise cross-validation. Numeric grids can be evaluated with selection.strategy = "sparse_kd".
selection.strategy	Candidate-selection strategy. "grid" evaluates the requested candidate grid. "sparse_kd" evaluates a sparse support-size by chart-dimension skeleton when chart.dim.grid is supplied. "plateau_kd" uses the same geometry-only support-size and chart-dimension plateau rule as fit.lps.
chart.dim.max	Optional explicit maximum chart dimension for the sparse coupled candidate family.
geometry.margin	Nonnegative integer subtracted from the local-PCA rank cap min(ncol(X), support.size - 1). The default zero applies only the Nadaraya–Watson chart-geometry requirement; this is not a local polynomial design margin.

`auto.chart.support.metric`
: Support system used by `chart.dim = "auto"` or `"local.auto"`. Chart-kernel smoothers currently use coordinate supports for both coordinate and operator diagnostics.

`auto.chart.selection.metric`
: Which auto chart-dimension diagnostic to use when both coordinate and operator summaries are requested.

`quadrature.weights`
: Optional positive reference-measure weights `q_i`. Defaults to unit weights.

`denominator.floor`
: Positive floor used when the local denominator is numerically zero.

`return.details` Logical; if `TRUE`, keep per-evaluation diagnostics.

Details

For an evaluation point x_u, the method chooses a local support U_u, builds either centered ambient coordinates or a local PCA chart, and computes

$$\widehat{f}(x_u) = \frac{\sum_{i \in U_u} y_i K_h(z_{ui})}{\sum_{i \in U_u} q_i K_h(z_{ui})}.$$

Here z_{ui} is the local chart coordinate of $x_i - x_u$, q_i is an optional quadrature weight, and K_h is the selected kernel.

Value

A list with class `"chart_kernel"` containing `fitted.values`, source/evaluation supports, selected controls, and denominator diagnostics.

Examples

```
X <- matrix(seq(0, 1, length.out = 21), ncol = 1)
y <- exp(-20 * (X[, 1] - 0.5)^2)
fit.chart.kernel(X, y, support.size = 7L, kernel = "gaussian")
```

---

fit.density *Fit a Density Estimator*

Description

Dispatches to a dedicated density estimator. Subject-occupation density estimation is one application: construct a sparse mass vector over a fixed support set and call this generic density layer.

Usage

```
fit.density(
  X,
  weights = NULL,
  method = c("empirical", "graph_random_walk"),
  graph = NULL,
  graph.control = list(),
  density.control = list(),
  return.details = TRUE,
  ...
)
```

Arguments

X	Numeric matrix with one row per support point.
weights	Optional nonnegative mass/count vector of length nrow(X). Required by count-based density methods.
method	Density method identifier.
graph	Optional precomputed graph object.
graph.control	List of graph-method controls.
density.control	List controlling clipping, normalization, and accounting checks. Recognized entries are mass.tol, neg.tol, clip.negative, and renormalize.
return.details	Logical; if TRUE, keep diagnostic details in the result.
...	Additional method-specific arguments.

Value

A list of class "density_fit" with fields method.id, status, rho, empirical.rho, fitted.raw, theta, accounting, smoothness, timing, diagnostics, and warnings.

Examples

```
X <- matrix(seq(0, 1, length.out = 6), ncol = 1)
fit.density(X, weights = c(1, 0, 2, 0, 0, 1), method = "empirical")
```

---

fit.graph.trend.filtering

Fit Graph Trend Filtering

Description

Fits graph trend filtering on a supplied undirected graph. Supported phase-2 orders are 0L, 1L, and 2L:

$$\widehat{\beta}_\lambda = \arg\min_{\beta \in \mathbb{R}^n} \left\{ \frac{1}{2}\|y - \beta\|_2^2 + \lambda \|\Delta_w^{(k+1)} \beta\|_1 \right\}.$$

Usage

```
fit.graph.trend.filtering(
  adj.list,
  weight.list = NULL,
  y,
  order = 0L,
  lambda.grid = NULL,
  lambda.selection = c("cv", "fixed"),
  weight.rule = c("conductance", "sqrt.conductance", "unit"),
  operator.family = c("graph.laplacian.recursive", "path.divided.difference"),
  path.family = c("branch.continuation", "all.simple"),
  path.weighting = c("unit", "anchor.mean"),
  n.lambda = 40L,
  nfolds = 5L,
  foldid = NULL,
  maxsteps = 2000L,
  minlam = 0,
  approx = FALSE,
  rtol = 1e-07,
  btol = 1e-07,
  eps = 1e-04,
  verbose = FALSE
)
```

Arguments

`adj.list`	List of integer neighbor vectors using 1-based vertex indices. The graph must be undirected: every edge must appear in both endpoint adjacency lists.
`weight.list`	Optional list of positive edge weights parallel to `adj.list`. For `operator.family = "graph.laplacian.recursive"`, weights are graph trend-filtering weights or conductances. For `operator.family = "path.divided.difference"`, weights are metric edge lengths used to define path coordinates. If `NULL`, all values are one.
`y`	Numeric response vector of length `length(adj.list)`.
`order`	Integer trend-filtering order. Supported values are `0L`, `1L`, and `2L`.
`lambda.grid`	Optional non-negative lambda grid. For `lambda.selection = "fixed"`, this must contain exactly one value. For `lambda.selection = "cv"`, `NULL` builds a default grid from the fitted full-data solution path.
`lambda.selection`	`"cv"` for vertex K-fold cross-validation or `"fixed"` for a supplied fixed lambda.
`weight.rule`	Character scalar. `"conductance"` uses `weight.list` directly as ω_e; `"sqrt.conductance"` uses $\sqrt{w_e}$; `"unit"` ignores `weight.list`. This applies to `operator.family = "graph.laplacian.recursive"`.
`operator.family`	Character scalar selecting the penalty operator family. The default `"graph.laplacian.recursive"` preserves the existing graph trend-filtering semantics. `"path.divided.difference"`

	uses local pathwise finite differences and is designed to reproduce classical one-dimensional trend filtering on path graphs.
`path.family`	Character scalar used for `operator.family = "path.divided.difference"`. `"branch.continuation"` keeps paths whose internal vertices do not pass through branch points. `"all.simple"` keeps all simple paths of the required length.
`path.weighting`	Character scalar used for `operator.family = "path.divided.difference"`. `"unit"` assigns every canonical path row weight one. `"anchor.mean"` divides rows by the number of retained canonical paths sharing the same canonical start vertex.
`n.lambda`	Number of default lambda candidates when `lambda.grid = NULL` and `lambda.selection = "cv"`.
`nfolds`	Number of CV folds.
`foldid`	Optional integer fold assignments of length `length(y)`.
`maxsteps`	Maximum number of path steps passed to **genlasso**.
`minlam`	Minimum lambda passed to **genlasso**.
`approx`	Logical; passed to **genlasso**.
`rtol`, `btol`, `eps`	Numerical controls passed to **genlasso**.
`verbose`	Logical. If `TRUE`, pass verbose output to **genlasso**.

Details

Graph trend filtering is intended as an ℓ_1-adaptive comparator to the ℓ_2 graph smoothers now housed in **geosmooth** and the legacy rdgraph comparator. The low-pass smoother penalizes broad quadratic graph roughness through a term like

$$\eta f^\top L f,$$

which shrinks high-frequency variation everywhere. Graph trend filtering instead penalizes absolute graph differences. For `order = 0L`, this is

$$\lambda \sum_e \omega_e |\beta_j - \beta_i|,$$

so many edge differences can become exactly zero while selected edges carry jumps. In this sense `order = 0L` is locally adaptive: fitted values can be piecewise constant over graph regions. Higher orders use

$$\Delta_w^{(1)} = D_w, \qquad \Delta_w^{(2)} = L_w, \qquad \Delta_w^{(3)} = D_w L_w,$$

with $L_w = D_w^\top D_w$.

The supplied `weight.list`, when used, is interpreted as a graph trend-filtering edge weight or conductance for `operator.family = "graph.laplacian.recursive"`. For `operator.family = "path.divided.difference"`, `weight.list` is interpreted as metric edge length and is used to form local path coordinates. Use `weight.rule = "sqrt.conductance"` when the recursive graph square-root convention is desired, and `weight.rule = "unit"` for an unweighted recursive graph fused-lasso penalty.

The solver backend is currently **genlasso**. Cross-validation refits the generalized-lasso problem on vertex-held-out training sets using a selection matrix X; this is useful for small and moderate diagnostic problems but is not yet a scalable production graph-trend-filtering solver.

Value

A list of class "graph.trend.filtering.fit" containing fitted values, residuals, selected lambda, the operator, path metadata, and CV diagnostics when requested.

References

Wang, Y.-X., Sharpnack, J., Smola, A., and Tibshirani, R. J. (2016). Trend filtering on graphs. *Journal of Machine Learning Research*, 17(105), 1–41. https://www.jmlr.org/papers/v17/15-147.html

Examples

```
if (requireNamespace("genlasso", quietly = TRUE)) {
  adj <- list(2L, c(1L, 3L), c(2L, 4L), 3L)
  fit.graph.trend.filtering(
    adj, y = c(0, 0.2, 1.8, 2), lambda.grid = 0.3,
    lambda.selection = "fixed", weight.rule = "unit"
  )
}
```

---

fit.local.likelihood *Fit a Local-Likelihood Density or Bernoulli Smoother*

Description

Fits a local likelihood model at each evaluation point and reads off one raw fitted value at that evaluation anchor. Density and Bernoulli workflows should convert the returned fitted field with normalize.density when the target is a subject-occupation density.

Usage

```
fit.local.likelihood(
  X,
  y,
  X.eval = NULL,
  likelihood.family = c("density", "bernoulli"),
  support.size = min(15L, nrow(X)),
  degree = 1L,
  kernel = c("gaussian", "tricube", "epanechnikov", "triangular"),
  bandwidth.multiplier = 1,
  support.grid = NULL,
  degree.grid = NULL,
  kernel.grid = NULL,
  bandwidth.multiplier.grid = NULL,
  lambda.ridge.grid = NULL,
  foldid = NULL,
  cv.folds = 5L,
```

```
  cv.seed = 1L,
  coordinate.method = c("coordinates", "local.pca"),
  chart.dim = NULL,
  chart.dim.grid = NULL,
  selection.strategy = c("grid", "sparse_kd", "plateau_kd"),
  chart.dim.max = NULL,
  design.margin = 2L,
  auto.chart.support.metric = c("coordinates", "operator", "both"),
  auto.chart.selection.metric = c("coordinates", "operator"),
  quadrature.weights = NULL,
  lambda.ridge = 1e-08,
  min.local.mass = sqrt(.Machine$double.eps),
  min.nonzero.mass = 1L,
  fallback = c("degree0", "zero", "chart_kernel", "na"),
  optimizer = c("newton", "optim"),
  max.iter = 50L,
  tol = 1e-08,
  return.details = TRUE
)
```

Arguments

`X`	Numeric matrix with one row per source/support point.
`y`	Numeric response vector. For `likelihood.family = "density"`, this must be a nonnegative mass/intensity vector with positive total mass. For `"bernoulli"`, values must lie in `[0, 1]`.
`X.eval`	Optional numeric matrix of evaluation points. Defaults to `X`.
`likelihood.family`	Local likelihood family.
`support.size`	Number of source points in each local support.
`degree`	Local chart feature degree. Supported values are 0, 1, and 2. The density branch omits an intercept because the intercept is not identifiable in the normalized local density likelihood. The Bernoulli branch includes an intercept in its internal logistic feature map.
`kernel`	Kernel name. Supported values are `"gaussian"`, `"tricube"`, `"epanechnikov"`, and `"triangular"`.
`bandwidth.multiplier`	Positive multiplier applied to the local support radius.
`support.grid`	Optional integer candidate neighborhood sizes for cross-validation. CV selection is currently implemented for `likelihood.family = "bernoulli"`.
`degree.grid`	Optional local polynomial degree candidates for Bernoulli cross-validation.
`kernel.grid`	Optional kernel candidates for Bernoulli cross-validation.
`bandwidth.multiplier.grid`	Optional bandwidth-multiplier candidates for Bernoulli cross-validation.
`lambda.ridge.grid`	Optional ridge-penalty candidates for Bernoulli cross-validation.

`foldid` Optional positive integer vector assigning source rows to cross-validation folds.

`cv.folds` Number of folds used when `foldid` is not supplied.

`cv.seed` Random seed used to generate folds when `foldid` is not supplied.

`coordinate.method`
: Local coordinate method. `"coordinates"` uses centered ambient coordinates. `"local.pca"` projects centered support points onto a local PCA basis.

`chart.dim` Local PCA dimension when `coordinate.method = "local.pca"`. If `NULL`, the dimension is `min(ncol(X), support.size - 1)`. The deployable input-only policies `"auto"` and `"local.auto"` use the same local-PCA dimension diagnostics as `fit.lps`; `"auto"` resolves one global chart dimension, while `"local.auto"` resolves one dimension per evaluation anchor.

`chart.dim.grid` Optional candidate chart dimensions for experimental cross-validation. Numeric grids can be evaluated with `selection.strategy = "sparse_kd"`.

`selection.strategy`
: Candidate-selection strategy. `"grid"` evaluates the requested candidate grid. `"sparse_kd"` evaluates a sparse support-size by chart-dimension skeleton when `chart.dim.grid` is supplied. `"plateau_kd"` uses the same geometry-only support-size and chart-dimension plateau rule as `fit.lps`.

`chart.dim.max` Optional explicit maximum chart dimension for the sparse coupled candidate family.

`design.margin` Nonnegative integer feasibility margin used to screen local polynomial design size before candidate evaluation.

`auto.chart.support.metric`
: Support system used by `chart.dim = "auto"` or `"local.auto"`. Local-likelihood smoothers currently use coordinate supports for both coordinate and operator diagnostics.

`auto.chart.selection.metric`
: Which auto chart-dimension diagnostic to use when both coordinate and operator summaries are requested.

`quadrature.weights`
: Optional positive reference-measure weights. Defaults to unit weights.

`lambda.ridge` Nonnegative ridge penalty on identifiable coefficients.

`min.local.mass` Minimum local kernel-weighted mass needed before attempting a higher-degree density fit. For Bernoulli fits this is used only as diagnostic telemetry.

`min.nonzero.mass`
: Minimum number of locally weighted positive-mass source points needed before attempting a higher-degree local fit.

`fallback` Fallback policy for underidentified or failed higher-degree local fits. Zero local mass always uses `"zero"`.

`optimizer` Optimizer for nonzero-degree density fits. `"newton"` is implemented; `"optim"` is accepted and delegates to BFGS.

`max.iter` Maximum optimizer iterations.

`tol` Convergence tolerance for gradient norm and step norm.

`return.details` Logical; if `TRUE`, keep per-evaluation diagnostics.

Details

The `likelihood.family = "density"` branch uses a local exponential tilt of the chart reference measure. The `"bernoulli"` branch uses a weighted local logistic likelihood and returns fitted probabilities at the evaluation anchors.

Value

A list with class `"local_likelihood"` containing `fitted.values`, selected controls, and local solver diagnostics.

Examples

```
X <- matrix(seq(0, 1, length.out = 21), ncol = 1)
y <- exp(-20 * (X[, 1] - 0.5)^2)
y <- y / sum(y)
fit.local.likelihood(X, y, likelihood.family = "density",
                     support.size = 7L, degree = 0L)
```

`fit.lpl.tf` *Fit A Local Polynomial Lifting Trend Filter*

Description

Fits the Phase-2 LPL-TF estimator with a fixed operator:

$$\hat{f} = \arg\min_{f} \frac{1}{2}\|y - f\|_2^2 + \lambda \|A_{\mathrm{LPL}} f\|_1.$$

Usage

```
fit.lpl.tf(
  X = NULL,
  y,
  operator = NULL,
  adj.list = NULL,
  weight.list = NULL,
  graph = NULL,
  degree = 2L,
  lambda.grid = NULL,
  lambda = NULL,
  lambda.selection = c("cv", "fixed"),
  operator.grid = NULL,
  foldid = NULL,
  cv.folds = 5L,
  cv.loss = c("mse", "rmse", "mae"),
  cv.seed = NULL,
  cv.repeats = 1L,
  solver = c("genlasso"),
```

```
  selection = c("min", "one.se"),
  n.lambda = 80L,
  maxsteps = 2000L,
  minlam = 0,
  approx = FALSE,
  rtol = 1e-07,
  btol = 1e-07,
  eps = 1e-04,
  verbose = FALSE,
  ...
)
```

Arguments

`X`	Optional coordinate matrix used to build `lpl.tf.operator` when `operator` is `NULL`.
`y`	Numeric response vector.
`operator`	Optional `"lpl_tf_operator"` object.
`adj.list`, `weight.list`, `graph`	Optional graph inputs passed to `lpl.tf.operator` when `operator` is `NULL`.
`degree`	Polynomial degree passed to `lpl.tf.operator` when `operator` is `NULL`.
`lambda.grid`	Optional nonnegative lambda grid.
`lambda`	Optional fixed lambda shortcut. If supplied, it is used as the single fixed lambda and `lambda.selection` must be `"fixed"`.
`lambda.selection`	`"cv"` or `"fixed"`. Phase 2 requires an explicit `lambda.grid` for CV so the candidate grid is not generated from the full response vector before fold scoring.
`operator.grid`	Optional Phase-3 operator candidate grid. Supply a data frame with one row per candidate or a list of named lists. Candidate fields may include operator-construction arguments such as `degree`, `support.type`, `support.size`, `min.support`, `support.buffer`, `kernel`, `row.normalize`, and `local.solver`.
`foldid`	Optional deterministic fold assignments for CV.
`cv.folds`	Number of generated folds when `foldid = NULL`.
`cv.loss`	Cross-validation loss, `"mse"`, `"rmse"`, or `"mae"`. `"rmse"` uses the same lambda ordering as MSE and reports square-rooted fold errors.
`cv.seed`	Reserved for reproducible generated folds. Phase 2 generated folds are deterministic even when this is `NULL`.
`cv.repeats`	Phase 2 supports only one CV repeat.
`solver`	Phase 2 supports only `"genlasso"`.
`selection`	Lambda selection rule, `"min"` or `"one.se"`.
`n.lambda`	Number of generated lambdas when a genlasso path is used and `lambda.grid = NULL`.
`maxsteps`, `minlam`, `approx`, `rtol`, `btol`, `eps`	Genlasso controls.

verbose	Logical.
...	Additional arguments passed to lpl.tf.operator when the operator is built internally.

Value

A list of class "lpl_tf".

Examples

```
if (requireNamespace("genlasso", quietly = TRUE)) {
  X <- matrix(seq(0, 1, length.out = 18), ncol = 1)
  fit.lpl.tf(X, sin(2 * pi * X[, 1]), degree = 1L,
             support.type = "knn", support.size = 7L,
             lambda = 0.1, lambda.selection = "fixed")
}
```

---

fit.lps *Fit a Local Polynomial Smoother*

Description

Fits a local polynomial smoother (LPS) and selects its support size, polynomial degree, and kernel by cross-validation. By default, the smoother works in the observed ambient coordinates: each prediction point uses its nearest training points in Euclidean distance, centers the support at the prediction point, fits a weighted local polynomial, and uses the fitted intercept as the prediction.

Usage

```
fit.lps(
  X,
  y,
  foldid = NULL,
  support.grid = c(10L, 15L, 20L),
  degree.grid = 0:2,
  kernel.grid = c("gaussian", "tricube"),
  cv.folds = 5L,
  cv.seed = 1L,
  X.eval = NULL,
  coordinate.method = c("coordinates", "local.pca"),
  chart.dim = NULL,
  chart.dim.grid = NULL,
  local.chart.method = c("pca", "second.order.svd"),
  auto.chart.support.metric = c("coordinates", "operator", "both"),
  auto.chart.selection.metric = c("coordinates", "operator"),
  backend = c("auto", "R", "cpp", "cpp.local.pca"),
  design.basis = c("orthogonal.polynomial.drop", "monomial", "weighted.qr",
    "weighted.qr.drop"),
```

```
  design.drop.tol = 1e-08,
  ridge.multiplier.grid = c(0, 1e-10, 1e-08),
  ridge.condition.max = 1e+12,
  unstable.action = c("na", "mean"),
  outcome.family = c("gaussian", "bernoulli", "binomial"),
  bandwidth.multiplier.grid = 1,
  keep.cv.predictions = FALSE,
  ridge.shrinkage.target = c("zero", "local.mean"),
  selection.strategy = c("grid", "sparse_kd", "plateau_kd"),
  chart.activation = c("none", "subject.od"),
  chart.activation.response = NULL,
  chart.activation.control = list(),
  chart.dim.max = NULL,
  design.margin = 2L
)
```

Arguments

X	Numeric design/coordinate matrix with one observation per row.
y	Numeric response vector with length nrow(X).
foldid	Optional positive integer vector assigning rows to CV folds.
support.grid	Integer candidate neighborhood sizes.
degree.grid	Integer polynomial degrees. Currently degrees 0, 1, and 2 are supported.
kernel.grid	Candidate kernels. Supported kernels are "gaussian", "tricube", "epanechnikov", and "triangular".
cv.folds	Number of folds used when foldid is not supplied.
cv.seed	Random seed used to generate folds when foldid is not supplied.
X.eval	Optional matrix of prediction locations. Defaults to X.
coordinate.method	Local coordinate system. "coordinates" uses centered ambient coordinates. "local.pca" uses a local PCA chart.
chart.dim	Chart dimension for coordinate.method = "local.pca". If NULL, defaults to ncol(X). The special value "auto" estimates one global chart dimension from observed X only. The experimental special value "local.auto" estimates a local chart dimension separately for each prediction anchor in the ordinary local-PCA R backend.
chart.dim.grid	Optional candidate chart dimensions for experimental coupled support-size by chart-dimension selection. When supplied, coordinate.method must be "local.pca" and the evaluated candidates use scalar numeric chart dimensions after feasibility filtering. The default NULL preserves the historical single-chart.dim behavior.
local.chart.method	Local chart constructor used when coordinate.method = "local.pca". "pca" preserves the ordinary local-PCA chart path. "second.order.svd" uses an experimental curvature-corrected second-order local SVD chart and records compact chart fallback diagnostics. This option is opt-in and does not affect ambient coordinate fits.

auto.chart.support.metric
: Support system used when chart.dim = "auto" or "local.auto". Included for consistency with LPL-TF and S-LPL-TF; because this smoother uses coordinate supports, "operator" is equivalent to "coordinates".

auto.chart.selection.metric
: Which auto chart-dimension diagnostic to select when both diagnostics are requested.

backend
: Computation backend. "auto" uses the C++ backend for coordinate.method = "coordinates" and the R reference backend for coordinate.method = "local.pca". "R" always uses the reference implementation. "cpp" requires ambient coordinates. "cpp.local.pca" is an opt-in prototype backend for coordinate.method = "local.pca" with local.chart.method = "pca".

design.basis
: Local polynomial design backend. "monomial" uses the ordinary raw monomial design. "weighted.qr" solves the same design using an explicit weighted-QR numerical path. "weighted.qr.drop" first drops numerically dependent local design columns by weighted QR before solving. "orthogonal.polynomial.drop" replaces the local monomial design by a weighted-orthogonal basis spanning its estimable polynomial directions, dropping numerically rank-deficient directions first.

design.drop.tol
: Relative QR tolerance used by design.basis = "weighted.qr.drop" or design.basis = "orthogonal.polynomial.drop".

ridge.multiplier.grid
: Nonnegative scale-relative ridge multipliers tried by the R local-solve backend. The smallest multiplier whose penalized local normal equations pass ridge.condition.max is used.

ridge.condition.max
: Maximum allowed condition number for the penalized local normal equations. Use Inf to disable this guard.

unstable.action
: Action when no local solve passes the rank and condition guards. "mean" preserves the historical weighted-mean fallback. "na" returns NA, causing CV candidates with unstable predictions to be avoided.

outcome.family
: Response family. "gaussian" preserves the ordinary numeric-response LPS behavior. "bernoulli" treats 0/1 responses as numeric conditional-expectation targets for $\Pr(Y = 1 \mid X)$, keeps the same local least-squares fitting core, clips reported response-scale probabilities to [0,1], selects candidates by the observed CV Brier score of the clipped predictions (E2.12: the selection score is the deployed metric, which requires per-point CV predictions, so "bernoulli" – like "binomial" – always uses the R backend: backend = "auto" resolves to "R" and an explicit C++ backend is an error), and records Brier/log-loss probability diagnostics. "binomial" uses local weighted logistic polynomial fits, selects candidates by observed CV log loss with the log-loss probability truncation pinned at 1e-6 (E2.12) and with any candidate having a non-finite CV prediction scored Inf – unselectable, the same rule as the gaussian/bernoulli selection scores (E2.15) – and reports probability diagnostics on the fitted probabilities. The local logistic IRLS uses deviance step-halving (E2.14): a Newton

update is accepted only if the weighted binomial deviance does not increase by more than 1e-8; otherwise the step is halved toward the current iterate (at most 30 times, after which the solve is declared non-convergent). The deviance is evaluated on the same [-35, 35] clamped linear predictor the IRLS update uses, so it is finite for every finite iterate. A solve that does not converge within the iteration cap (including under exact separation, where the unpenalized logistic MLE does not exist) falls back deterministically to the local weighted event rate under unstable.action = "mean" or to NA under unstable.action = "na"; every fallback is counted in logistic.diagnostics (fallback.path, event.rate.fallback, na.failure).

bandwidth.multiplier.grid

Nonnegative bandwidth multipliers added to the CV candidate grid. For a candidate with multiplier b, the local kernel bandwidth becomes $h = b \cdot d_{(K)}$ where $d_{(K)}$ is the distance to the K-th nearest support neighbor, decoupling the kernel scale from the support size. The default 1 reproduces the historical behavior exactly (the bandwidth equals the support radius). Any grid other than exactly 1 requires the R reference backend: backend = "auto" then resolves to "R", and explicit backend = "cpp" or "cpp.local.pca" is an error. The selected multiplier is returned in $selected$bandwidth.multiplier and as a bandwidth.multiplier column of cv.table.

keep.cv.predictions

Logical; if TRUE, the returned object additionally carries cv.predictions, the matrix of out-of-fold CV predictions with one column per cv.table row, so selection scores can be recomputed from the actual CV predictions (E2.12). NULL on the C++ CV paths (reachable only for outcome.family = "gaussian"), which do not materialize per-point predictions. Default FALSE leaves the returned object exactly as before.

ridge.shrinkage.target

Shrinkage target of the local ridge penalty in the least-squares solve (E2.13). The default "zero" preserves the historical behavior bit-for-bit: in the orthogonal design bases the penalty acts on every transformed direction, including the constant, so a large ridge multiplier shrinks the local prediction toward 0. "local.mean" – the statistically recommended setting – leaves the constant direction unpenalized via a weighted-centering reparametrization, so a large ridge shrinks the prediction toward the local weighted mean instead, and rho = 0 remains the unpenalized weighted least-squares solve. The two settings coincide for the non-orthogonal design bases ("monomial", "weighted.qr", "weighted.qr.drop"), whose constant column is already unpenalized, and at rho = 0. The setting applies to the least-squares solve (outcome.family "gaussian" / "bernoulli"); it has *no effect* on the "binomial" local logistic solver, whose ridge keeps the historical structure (a warning is issued if combined).

selection.strategy

Candidate-selection strategy. "grid" preserves the full Cartesian candidate grid. The experimental "sparse_kd" strategy evaluates a sparse coupled support-size by chart-dimension skeleton when chart.dim.grid is supplied. "plateau_kd" is a geometry-only selector: from observed X only, it estimates the local PCA variance dimension over the supplied support grid, finds the initial support-size plateau where that dimension is stable from the smallest support size, aggregates

plateau endpoints across representative anchors, and evaluates the resulting single (support.size, chart.dim) candidate.

chart.activation
: Optional sparse-response chart activation rule. "none" preserves the ordinary LPS behavior. "subject.od" is intended for subject-occupation density workflows: a local chart whose support contains too little subject occupation mass, too few positive subject-visited points, or only fringe occupation receives fitted value zero without constructing the local polynomial fit.

chart.activation.response
: Optional nonnegative response used only by chart.activation = "subject.od" to decide whether a chart is active. When omitted, y is used.

chart.activation.control
: List controlling sparse chart activation. Supported fields are mass.min, n.positive.min, positive.tol, core.weight.rule, core.weight.quantile, and core.weight.min. The OD default is two positive support points and a chart-specific 0.25 weight quantile.

chart.dim.max
: Optional explicit maximum chart dimension for the experimental coupled selector.

design.margin
: Nonnegative prefit margin used to mark coupled (support.size, chart.dim) candidates infeasible when the full local polynomial design would be underdetermined.

Details

The optional coordinate.method = "local.pca" mode keeps the same support and kernel weighting rule, but builds the local polynomial in a local PCA chart centered at each prediction point. With chart.dim = "auto", the chart dimension is estimated as one global scalar from observed X only, using the same shared local-PCA dimension helper used by LPL-TF and S-LPL-TF. The experimental chart.dim = "local.auto" mode estimates an input-only local chart dimension separately for each prediction anchor.

Value

A list of class "lps" with response-scale fitted.values, unmodified local least-squares fitted.values.raw, selected parameters, a candidate CV table, the requested local.chart.method, and the effective chart method used for reporting. In outcome.family = "bernoulli" or "binomial" mode, fitted.values are response-scale probabilities in [0,1], fitted.values.raw are the un-clipped conditional-expectation estimates for "bernoulli" and the fitted probabilities for "binomial", cv.table$cv.brier.observed is the observed CV Brier score of the response-scale (clipped) predictions with Inf for candidates having any non-finite prediction, and probability.diagnostics records raw/clipped probability ranges, out-of-range fractions, and Brier/log-loss diagnostics. The Brier and log-loss diagnostics are defined only when the fitted predictions have the same length as the training response, which is the default X.eval = X path. In "binomial" mode, logistic.diagnostics records local logistic solve attempts, convergence statuses, fallback-path counts, event-rate fallback counts, and NA failure counts separately for CV and final fitting.

References

Fan, J. and Gijbels, I. (1996). *Local Polynomial Modelling and Its Applications*. Chapman and Hall/CRC. ISBN 9780412983214.

Examples

```
X <- matrix(seq(0, 1, length.out = 20), ncol = 1)
y <- sin(2 * pi * X[, 1])
fit <- fit.lps(
  X, y, support.grid = 8L, degree.grid = 1L,
  kernel.grid = "tricube", cv.folds = 2L, backend = "R"
)
head(fit$fitted.values)
```

`fit.malps` *Fit Model-Averaged Local Polynomial Smoothing*

Description

Fits the current model-averaged local polynomial smoother (MALPS) on a supplied coordinate matrix. MALPS fits local polynomial regressions around observed anchor points and averages all positive-weight local predictions at each training point. The current implementation supports supplied coordinates, observed or supplied coordinate anchors, fixed support parameters, deterministic cross-validation and exact dense GCV over support parameters, local PCA chart coordinates, ordinary and weighted new-response refits, coordinate-space new-point prediction, linear-smoother diagnostics, and fixed-selection bootstrap uncertainty summaries. Graph-geodesic supports are available for training and refit; graph-geodesic new-point prediction is deferred.

Usage

```
fit.malps(
  X,
  y,
  graph = NULL,
  adj.list = NULL,
  weight.list = NULL,
  graph.stage = "final",
  anchor.index = NULL,
  anchor.coordinates = NULL,
  degree = 2L,
  degree.grid = NULL,
  support.type = c("adaptive.radius", "knn", "fixed.radius"),
  support.size = NULL,
  support.grid = NULL,
  radius = NULL,
  radius.grid = NULL,
  min.support = NULL,
```

```
  min.support.grid = NULL,
  support.buffer = 3L,
  kernel = c("epanechnikov", "triangular", "gaussian", "tricube"),
  kernel.grid = NULL,
  model.weight.rule = c("none", "condition", "support", "boundary", "quality"),
  duplicate.action = c("keep", "error"),
  coordinate.method = c("coordinates", "local.pca"),
  chart.dim = NULL,
  support.metric = c("auto", "coordinates", "graph.geodesic"),
  auto.chart.support.metric = c("coordinates", "operator", "both"),
  auto.chart.selection.metric = c("coordinates", "operator"),
  support.selection = c("fixed", "cv", "gcv"),
  foldid = NULL,
  cv.folds = 5L,
  cv.loss = c("rmse", "mae", "mse"),
  cv.repeats = 1L,
  cv.seed = NULL,
  cv.one.se = FALSE,
  gcv.exact.max.n = 1000L,
  local.solver = c("auto", "normal.equations", "qr", "svd"),
  normal.equations.max.condition = 1e+08,
  robust.iterations = 0L,
  robust.tuning.constant = 6,
  verbose = FALSE,
  ...
)
```

Arguments

X	Numeric coordinate matrix with one row per observation.
y	Numeric response vector with length nrow(X).
graph	Optional supported **dgraphs** graph object, for example from dgraphs::create.rknn.graph(). When support.metric = "graph.geodesic" or "auto" with a graph supplied, weighted shortest-path distances from this graph are used for support construction.
adj.list	Optional 1-based undirected adjacency list. Must be supplied together with weight.list when using a supplied graph payload.
weight.list	Optional positive edge-length list parallel to adj.list. Edge weights are interpreted as graph lengths.
graph.stage	Graph lifecycle stage used when graph is a **dgraphs** graph object. Supported stages include "final", "raw", and "pruned" when those payloads are available on the supplied graph.
anchor.index	Optional integer vector of observed rows used as local model anchors. Defaults to all rows when anchor.coordinates is NULL.
anchor.coordinates	Optional numeric coordinate matrix of off-sample local model anchors with the same number of columns as X. This option is currently supported only with coordinate support distances, not with support.metric = "graph.geodesic".

`degree` Local polynomial degree, one of `0L`, `1L`, or `2L`.

`degree.grid` Optional degree grid used when `support.selection` is `"cv"` or `"gcv"`.

`support.type` Support construction rule. `"knn"` uses exactly `support.size` nearest observations including the anchor itself for full-data local fitting supports. Prediction supports are then rebuilt from the induced local radius, so tied targets at the kNN boundary can be covered even when they were not part of the exact-size fitting support. `"adaptive.radius"` uses a radius large enough to include at least `min.support` observations. `"fixed.radius"` uses the supplied `radius`.

`support.size` Number of nearest observations for `support.type = "knn"`. If `NULL`, defaults to `min.support`.

`support.grid` Optional kNN support-size grid used when `support.selection` is `"cv"` or `"gcv"`.

`radius` Radius for `support.type = "fixed.radius"` and optional base radius for `support.type = "adaptive.radius"`.

`radius.grid` Optional radius grid used when `support.selection` is `"cv"` or `"gcv"`.

`min.support` Minimum positive-weight support size. If `NULL`, defaults to the local polynomial design size plus `support.buffer`.

`min.support.grid` Optional minimum-support grid used when `support.selection` is `"cv"` or `"gcv"`.

`support.buffer` Nonnegative integer added to the local design size when deriving the default `min.support`.

`kernel` Kernel used for local fitting and model averaging.

`kernel.grid` Optional kernel grid used when `support.selection` is `"cv"` or `"gcv"`.

`model.weight.rule` Optional per-anchor model-quality multiplier applied to the ordinary kernel averaging weights. `"none"` preserves the kernel-only averaging from earlier phases. `"condition"` downweights poorly conditioned local designs with $q_u^{\mathrm{cond}} = 1/\max(\kappa_u, 1)$. `"support"` upweights anchors with larger positive fitting supports using support size divided by the maximum support size. `"boundary"` downweights asymmetric boundary-like supports with $q_u^{\mathrm{bdry}} = 1/(1+b_u)$. `"quality"` multiplies these three component weights. For every non-`"none"` rule, `diagnostics$model.weight.raw` stores the selected unnormalized rule multiplier, while `model.weights` and `diagnostics$model.weight` store the final multipliers after median-one normalization over positive raw values. Raw zero or non-finite multipliers are retained diagnostically but are replaced by a tiny positive final floor before prediction averaging, so model-quality rules reweight existing prediction support rather than removing anchors from support membership. These weights affect prediction averaging only; they do not change local supports or local coefficient estimation.

`duplicate.action` How duplicate coordinate rows should be handled. `"keep"` allows duplicates, records duplicate diagnostics, and preserves observed-anchor self-inclusion. `"error"` rejects duplicate rows. Jittering duplicates is deliberately not implemented in Phase 1.

coordinate.method
: Coordinate system used for each local polynomial design. "coordinates" uses supplied coordinates centered at the anchor. "local.pca" uses a deterministic local PCA chart estimated from the anchor support.

chart.dim
: Local chart dimension for coordinate.method = "local.pca". If NULL, defaults to ncol(X). The special value "auto" estimates a single observed-data local PCA dimension without using responses, truth values, latent coordinates, or labels. For coordinate.method = "coordinates", chart.dim must be NULL.

support.metric
: Distance system used for support construction. "coordinates" uses Euclidean distances in X. "graph.geodesic" uses weighted shortest-path distances from graph or adj.list/weight.list. "auto" uses graph geodesic distances when graph input is supplied and coordinate distances otherwise.

auto.chart.support.metric
: Support system used when chart.dim = "auto". "coordinates" uses Euclidean coordinate neighborhoods, "operator" uses the resolved MALPS support metric, and "both" computes both diagnostics side by side.

auto.chart.selection.metric
: Which auto chart-dimension diagnostic to use for the fitted MALPS model when both diagnostics are available. The default "coordinates" preserves historical behavior.

support.selection
: "fixed" for a single support profile, "cv" to tune support parameters by cross-validation, or "gcv" to tune support parameters by exact dense generalized cross-validation. The GCV path is cached across candidates and is exact for fixed-weight linear MALPS fits; it rejects robust residual reweighting.

foldid
: Optional integer fold assignments. If supplied, cv.repeats is forced to one.

cv.folds
: Number of folds generated when foldid = NULL.

cv.loss
: Cross-validation loss.

cv.repeats
: Number of independent fold assignments generated when foldid = NULL.

cv.seed
: Optional seed for generated folds.

cv.one.se
: Logical; use a one-standard-error rule for support selection.

gcv.exact.max.n
: Maximum number of observations allowed for exact dense GCV support selection. Larger datasets should use "cv" until a sparse or trace-estimated GCV path is implemented.

local.solver
: Local weighted least-squares solver. "auto" uses normal equations only for full-rank, well-conditioned local designs and otherwise falls back to SVD.

normal.equations.max.condition
: Maximum local design condition number for normal equations under local.solver = "auto".

robust.iterations
: Number of Cleveland-style robust residual reweighting iterations applied inside each local polynomial fit. The default 0L preserves ordinary MALPS. Positive values multiply the geometric fitting weights by Tukey bisquare residual weights recomputed from the local fit.

`robust.tuning.constant`
: Positive bisquare tuning constant. The default `6` matches the usual LOWESS convention in which residuals are scaled by `6 * median(abs(residuals))`.

`verbose`
: Logical; reserved for future progress messages.

`...`
: Reserved for future extensions. Supplying unused arguments is an error.

Details

Current development benchmarks suggest using the plain MALPS defaults for production-style fits unless a specific diagnostic motivates a non-default option: `support.selection = "cv"`, `robust.iterations = 0L`, `model.weight.rule = "none"`, and observed anchors (`anchor.coordinates = NULL`). Exact GCV selection (`support.selection = "gcv"`) is a useful faster option for fixed-weight, non-robust MALPS fits, especially exploratory continuous smoothing runs, but it is not yet the universal default. Binary responses are treated as numeric conditional-expectation targets; fitted values are not clipped inside the smoother. Grid anchors, empirical-Bayes shrinkage, robust local residual reweighting, and conservative/smoothed GCV selection remain experimental controls rather than default recommendations.

Graph construction is supplied by **dgraphs** or by explicit `adj.list`/`weight.list` payloads. Coordinate MALPS paths and graph-geodesic payload validation are package-local; shortest-path distances are computed through **dgraphs**.

Value

A list of class `"malps"` with fitted values, local model coefficients, supports, averaging weights, diagnostics, and selection metadata.

Examples

```
X <- matrix(seq(0, 1, length.out = 20), ncol = 1)
fit <- fit.malps(X, sin(2 * pi * X[, 1]), degree = 1L,
                 support.type = "knn", support.size = 8L)
head(fit$fitted.values)
```

---

fit.metric.graph.lowpass

Fit Metric-Conductance Graph Low-Pass Regression

Description

Fits graph-spectral low-pass regression on a supplied graph by transforming metric edge lengths into conductances and smoothing the response in the eigenbasis of the weighted graph Laplacian.

Usage

```
fit.metric.graph.lowpass(
  adj.list,
  weight.list,
  y,
  conductance.rule = c("inverse.length.power", "exp.length", "exp.length.squared",
    "self.tuned.gaussian"),
  conductance.epsilon = 1e-08,
  conductance.alpha = 1,
  conductance.sigma = NULL,
  conductance.sigma.rule = c("edge.quantile", "median", "local.k"),
  conductance.sigma.quantile = 0.75,
  conductance.local.k = 5L,
  laplacian.type = c("unnormalized", "symmetric.normalized"),
  n.eigenpairs = 50L,
  filter.type = c("heat_kernel", "tikhonov", "cubic_spline", "gaussian", "exponential",
    "butterworth"),
  eta.grid = NULL,
  n.candidates = 40L,
  eigen.solver = c("auto", "sparse", "dense"),
  dense.eigen.threshold = 200L,
  dense.fallback.threshold = 5000L,
  dense.fallback = c("auto", "never", "always"),
  verbose = FALSE,
  eta.search = c("fixed", "guarded.gcv"),
  eta.expansion.factor = 3,
  eta.max.expansions = 3L,
  eta.identity.departure = 0.01,
  eta.truncation.tol = 1e-04
)
```

Arguments

`adj.list`	List of integer neighbor vectors using 1-based vertex indices.
`weight.list`	List of positive metric edge lengths parallel to `adj.list`. These are interpreted as edge lengths, not conductances.
`y`	Numeric response vector of length `length(adj.list)`.
`conductance.rule`	Character scalar. One of `"inverse.length.power"`, `"exp.length"`, `"exp.length.squared"`, or `"self.tuned.gaussian"`.
`conductance.epsilon`	Positive numeric regularizer used by inverse-power conductances and as a local-scale floor.
`conductance.alpha`	Positive numeric exponent for `"inverse.length.power"`.
`conductance.sigma`	Optional positive global scale for exponential rules. If `NULL`, it is selected by `conductance.sigma.rule`.

`conductance.sigma.rule`
: Rule for selecting a global scale when needed.

`conductance.sigma.quantile`
: Quantile used when `conductance.sigma.rule = "edge.quantile"`.

`conductance.local.k`
: Positive integer local incident-edge order statistic for `"self.tuned.gaussian"`.

`laplacian.type`
: Laplacian operator. `"unnormalized"` uses the weighted graph Laplacian $L = D - C$. `"symmetric.normalized"` uses $L_{\mathrm{sym}} = I - D^{-1/2} C D^{-1/2}$.

`n.eigenpairs`
: Positive integer number of eigenpairs to compute.

`filter.type`
: Spectral low-pass filter family.

`eta.grid`
: Optional numeric eta grid. Values must be positive except for `filter.type = "heat_kernel"`, where `eta = 0` is allowed and gives the identity/no-smoothing limit. If `NULL`, the existing package helper `generate.eta.grid()` is used.

`n.candidates`
: Number of eta candidates when `eta.grid = NULL`.

`eigen.solver`
: `"auto"`, `"sparse"`, or `"dense"`. `"auto"` uses dense decomposition only for `n <= dense.eigen.threshold`, then sparse-first.

`dense.eigen.threshold`
: Exact dense threshold for auto mode. Default `200L`, intended for small reference/testing problems.

`dense.fallback.threshold`
: Maximum graph size for emergency dense fallback when sparse decomposition fails and fallback is allowed.

`dense.fallback`
: `"auto"`, `"never"`, or `"always"`.

`verbose`
: Logical. Reserved for future diagnostic messages.

`eta.search`
: Heat-time search controller. `"fixed"` evaluates the supplied or generated grid once. `"guarded.gcv"` is available only for `filter.type = "heat_kernel"` and proposes one lower positive time whenever GCV selects the current lower endpoint.

`eta.expansion.factor`
: Geometric divisor used by guarded GCV lower-time expansion.

`eta.max.expansions`
: Maximum number of guarded GCV lower-time extensions.

`eta.identity.departure`
: Smallest allowed departure from the identity at the largest retained graph-Laplacian eigenvalue.

`eta.truncation.tol`
: Omitted-mode attenuation tolerance used to certify guarded proposals for a truncated basis.

Value

A list of class `"metric.graph.lowpass.fit"`.

References

Gajer, P. and Ravel, J. (2025). Adaptive geometric regression for high-dimensional structured data. arXiv:2511.03817. doi:10.48550/arXiv.2511.03817

Examples

```
adj <- list(2L, c(1L, 3L), c(2L, 4L), 3L)
lengths <- list(1, c(1, 1), c(1, 1), 1)
fit.metric.graph.lowpass(
  adj, lengths, y = c(0, 0.2, 1.8, 2), n.eigenpairs = 4L,
  eta.grid = c(0.1, 1), eigen.solver = "dense"
)
```

`fit.ps.lps` *Fit Prediction-Synchronized Local Polynomial Smoothing*

Description

Experimental R reference implementation of prediction-synchronized local polynomial smoothing (PS-LPS). For fixed local polynomial parameters, PS-LPS fits one local polynomial chart per anchor and adds a quadratic penalty that synchronizes chart predictions on overlap points.

Usage

```
fit.ps.lps(
  X,
  y,
  foldid = NULL,
  support.size = NULL,
  degree = 2L,
  kernel = "gaussian",
  chart.dim = NULL,
  support.grid = NULL,
  degree.grid = NULL,
  kernel.grid = NULL,
  auto.chart.support.metric = c("coordinates", "operator", "both"),
  auto.chart.selection.metric = c("coordinates", "operator"),
  chart.dim.grid = NULL,
  selection.strategy = c("grid", "sparse_kd", "plateau_kd"),
  chart.dim.max = NULL,
  design.margin = 2L,
  lambda.sync.grid = c(0, 0.001, 0.01, 0.1, 1, 10),
  lambda.sync.search = c("grid", "guarded"),
  lambda.sync.selection = c("cv", "fixed"),
  local.candidate.search = c("screened", "full", "subgrid"),
  local.candidate.search.control = list(),
  lambda.sync.search.control = list(),
```

```
  lambda.diagnostics = c("all", "selected"),
  lambda.ridge = 1e-08,
  design.basis = c("monomial", "weighted.qr", "weighted.qr.drop",
    "orthogonal.polynomial.drop"),
  design.drop.tol = sqrt(.Machine$double.eps),
  ridge.multiplier.grid = NULL,
  ridge.condition.max = Inf,
  sync.neighbor.size = NULL,
  overlap.weight = c("normalized.product", "product"),
  chart.activation = c("none", "subject.od"),
  chart.activation.response = NULL,
  chart.activation.control = list(),
  ps.lps.geometry.cache = NULL,
  ps.lps.local.pca.supports = NULL,
  cv.folds = 5L,
  cv.seed = 1L
)
```

Arguments

`X`	Numeric covariate matrix.
`y`	Numeric response vector.
`foldid`	Optional integer cross-validation fold assignment.
`support.size`	Optional single neighborhood size for the fixed local setup path. Use `support.grid` for CV selection over neighborhood sizes.
`degree`	Single local polynomial degree for the fixed local setup path. Use `degree.grid` for CV selection over degrees.
`kernel`	Single kernel name for the fixed local setup path. Use `kernel.grid` for CV selection over kernels.
`chart.dim`	Chart dimension for the local PCA charts. A scalar fixes one dimension for all anchors; an integer vector supplies one local chart dimension per anchor. The special value `"auto"` estimates one global chart dimension from observed `X` only. The experimental special value `"local.auto"` estimates one local chart dimension per anchor, using the same local-PCA dimension rule as `fit.lps`.
`support.grid`	Candidate neighborhood sizes. When supplied, PS-LPS selects over support size, degree, kernel, and synchronization strength by materialized-fold CV. If both `support.size` and `support.grid` are absent, defaults to `c(10L, 15L, 20L)`, matching `fit.lps`.
`degree.grid`	Candidate local polynomial degrees for grid selection. Defaults to the scalar `degree`.
`kernel.grid`	Candidate kernels for grid selection. Defaults to the scalar `kernel`.
`auto.chart.support.metric`	Support system used when `chart.dim = "auto"` or `"local.auto"`. Because PS-LPS uses coordinate supports, `"operator"` is equivalent to `"coordinates"`.
`auto.chart.selection.metric`	Which auto chart-dimension diagnostic to select when both diagnostics are requested.

`chart.dim.grid` Optional candidate chart dimensions for experimental local-candidate selection. Numeric grids can be evaluated with `selection.strategy = "sparse_kd"`.

`selection.strategy`
Candidate-selection strategy. `"grid"` evaluates the requested candidate grid. `"sparse_kd"` evaluates a sparse support-size by chart-dimension skeleton when `chart.dim.grid` is supplied. `"plateau_kd"` uses the same geometry-only support-size and chart-dimension plateau rule as `fit.lps`.

`chart.dim.max` Optional explicit maximum chart dimension for the sparse coupled candidate family.

`design.margin` Nonnegative integer feasibility margin used to screen local polynomial design size before candidate evaluation.

`lambda.sync.grid`
Candidate synchronization strengths.

`lambda.sync.search`
Lambda-search policy. `"grid"` evaluates the supplied grid exactly. `"guarded"` uses an experimental guarded coarse-to-refine search with boundary expansion.

`lambda.sync.selection`
Lambda-selection mode. `"cv"` performs the usual internal fold-weighted lambda selection. `"fixed"` treats the single value in `lambda.sync.grid` as preselected and skips internal lambda CV; this is intended for outer selection loops that already score scalar candidates.

`local.candidate.search`
Local-candidate search policy when `support.grid`, `degree.grid`, or `kernel.grid` contains more than one candidate. `"screened"` is the routine default: it first ranks candidates by ordinary LPS materialized-fold CV, then runs PS-LPS only on a screened subset plus guard candidates. `"full"` evaluates PS-LPS lambda search for every local candidate and is the exact audit/reference path. `"subgrid"` skips the ordinary-LPS screening pass and evaluates only a deterministic support/kernel guard subgrid; this is intended for high-dimensional preflight runs where the screening pass is itself too expensive.

`local.candidate.search.control`
Optional list controlling screened local-candidate search. Supported fields are `top.n` (default 8), `max.candidates` (default 12), `neighbor.radius` (default 1), and `guard.support.quantiles` (default `c(0, 0.5, 1)`).

`lambda.sync.search.control`
Optional list controlling guarded search. Supported fields are `coarse.size` (default 5), `refine.radius` (default 2), `rel.tol` (default `0.002`), `boundary.guard.rel.tol` (default `0.01`), `boundary.expand` (default `TRUE`), `boundary.factor` (default 3), `max.boundary.expansions` (default 2), and `max.candidates` (default 25). Boundary expansion may evaluate positive candidates outside the supplied `lambda.sync.grid`. `max.candidates` is a global cap on distinct evaluated candidates; a very small cap can prevent local refinement or boundary expansion.

`lambda.diagnostics`
Lambda-diagnostic evaluation policy. `"all"` computes synchronization-energy and local-GCV diagnostics for every evaluated lambda and is the audit/reference mode. `"selected"` computes those diagnostics only for the selected lambda, which is faster for routine selection.

`lambda.ridge` Nonnegative scale-relative ridge used in the chart coefficient solve. Use `0` for the unregularized least-squares model.

`design.basis` Local polynomial design backend. See `fit.lps`. In PS-LPS, `"weighted.qr.drop"` drops numerically dependent columns separately in each anchor chart before the synchronized system is assembled, and `"orthogonal.polynomial.drop"` builds each synchronized chart in a weighted-orthogonal polynomial basis.

`design.drop.tol`
Relative QR tolerance used by `design.basis = "weighted.qr.drop"` or `design.basis = "orthogonal.polynomial.drop"`.

`ridge.multiplier.grid`
Optional nonnegative ridge multipliers for adaptive scale-relative ridge selection. When supplied, the solver uses the smallest multiplier whose penalized normal equations pass `ridge.condition.max`. If `NULL`, `lambda.ridge` is used as the single multiplier for backward compatibility.

`ridge.condition.max`
Maximum allowed condition number for adaptive ridge selection. Use `Inf` to disable the condition-number guard.

`sync.neighbor.size`
Number of nearby anchor pairs considered for synchronization from each anchor support.

`overlap.weight` Overlap weighting rule.

`chart.activation`
Optional sparse-response chart activation rule. `"none"` preserves ordinary PS-LPS. `"subject.od"` is intended for subject-occupation density workflows and deactivates local charts with no subject mass, too few positive subject-visited support points, or only fringe occupation.

`chart.activation.response`
Optional nonnegative vector used only for `chart.activation = "subject.od"` to decide whether each chart is active. When omitted, `y` is used.

`chart.activation.control`
List controlling sparse chart activation; see `fit.lps`.

`ps.lps.geometry.cache`
Optional precomputed geometry cache used by occupation-density cross-validation. This is an implementation detail; ordinary callers should leave it as `NULL`.

`ps.lps.local.pca.supports`
Optional precomputed local-PCA supports used when activation-specific frames must be rebuilt. This is an implementation detail; ordinary callers should leave it as `NULL`.

`cv.folds` Number of folds when `foldid` is absent.

`cv.seed` Fold seed when `foldid` is absent.

Value

A list with fitted values, selected lambda, CV table, diagnostics, and fitted chart coefficients.

Examples

```
X <- matrix(seq(0, 1, length.out = 20), ncol = 1)
fit.ps.lps(
  X, sin(2 * pi * X[, 1]), support.size = 7L, degree = 1L,
  chart.dim = 1L, lambda.sync.grid = 0,
  lambda.sync.selection = "fixed", cv.folds = 2L
)
```

`fit.pttf.trend.filtering` *Fit A Parallel-Transport Trend Filter From A PTTF Operator*

Description

Fits the first experimental PTTF regression models from a transported difference operator produced by `pttf.operator`. Phase 3 focuses on one response vector and explicit operator-row policies, especially the 1-D boundary policy used to separate interior transported rows from endpoint rows.

Usage

```
fit.pttf.trend.filtering(
  geometry = NULL,
  operator = NULL,
  X = NULL,
  y,
  derivative.order = 3L,
  penalty = c("l1", "l2"),
  lambda.grid = NULL,
  lambda.selection = c("cv", "fixed"),
  n.lambda = 80L,
  nfolds = 5L,
  foldid = NULL,
  cv.loss = c("mse", "mae"),
  selection = c("min", "one.se"),
  lambda.extension = c("none", "auto"),
  solver = c("genlasso", "admm", "auto"),
  operator.row.policy = c("all", "drop.line.boundary", "diagnostic.only"),
  line.order = NULL,
  boundary.trim = NULL,
  row.mass.rule = c("none", "node.mass"),
  row.normalize = c("none", "l2"),
  weights = NULL,
  maxsteps = 2000L,
  minlam = 0,
  approx = FALSE,
  rtol = 1e-07,
  btol = 1e-07,
```

```
  eps = 1e-04,
  admm.rho = 1,
  admm.maxiter = 2000L,
  admm.abstol = 1e-04,
  admm.reltol = 0.001,
  verbose = FALSE,
  ...
)
```

Arguments

`geometry`	Optional `"pttf_geometry"` object. Used only when `operator` is `NULL`.
`operator`	Optional `"pttf_operator"` object. Supplying an operator is recommended for validation so geometry/operator construction is separated from fitting.
`X`	Optional data matrix used to build `pttf.geometry` when both `geometry` and `operator` are `NULL`.
`y`	Numeric response vector.
`derivative.order`	Integer derivative order passed to `pttf.operator` when an operator must be built.
`penalty`	`"l1"` for generalized-lasso style fitting or `"l2"` for the quadratic energy fit.
`lambda.grid`	Optional lambda grid. Required for `lambda.selection = "fixed"`.
`lambda.selection`	`"cv"` or `"fixed"`.
`n.lambda`	Number of lambdas in a generated grid.
`nfolds`	Number of folds used only when `foldid = NULL`.
`foldid`	Optional integer fold assignments. Validation lanes should pass a materialized `foldid`; otherwise folds are generated by R's current RNG state.
`cv.loss`	Cross-validation loss, `"mse"` or `"mae"`.
`selection`	Lambda selection rule, `"min"` or `"one.se"`.
`lambda.extension`	Currently recorded as metadata. Phase 3 implements no new extension heuristic.
`solver`	L1 solver backend.
`operator.row.policy`	Which operator rows to use for fitting.
`line.order`	Vertex order for 1-D boundary-row policies.
`boundary.trim`	Number of endpoint ranks to drop for `operator.row.policy = "drop.line.boundary"`. Defaults to `derivative.order`.
`row.mass.rule, row.normalize`	Passed to `pttf.operator` when this function builds an operator. `row.normalize` is also used as the L1 solver row scaling for the supplied fit operator.
`weights`	Optional nonnegative observation weights.
`maxsteps, minlam, approx, rtol, btol, eps`	Genlasso controls for L1 fits.

admm.rho, admm.maxiter, admm.abstol, admm.reltol
: ADMM controls used when the L1 backend is "admm" or falls back to ADMM.

verbose
: Logical.

...
: Additional arguments passed to pttf.geometry or pttf.operator when those objects are built internally.

Value

A list of class "pttf.trend.filtering.fit".

Examples

```
n <- 10L
X <- matrix(seq(0, 1, length.out = n), ncol = 1)
adj <- lapply(seq_len(n), function(i) intersect(c(i - 1L, i + 1L), 1:n))
lengths <- Map(function(i, j) abs(X[j, 1] - X[i, 1]), seq_len(n), adj)
geometry <- pttf.geometry(
  X, adj, lengths, graph = "supplied", tangent.dim = 1L
)
operator <- pttf.operator(geometry, derivative.order = 2L)
fit.pttf.trend.filtering(
  operator = operator, y = sin(2 * pi * X[, 1]), penalty = "l2",
  lambda.grid = 0.1, lambda.selection = "fixed"
)
```

---

fit.slpl.tf *Fit A Fixed-Operator Synchronized LPL-TF Model*

Description

Fits the fixed-operator S-LPL-TF estimator

$$\hat{f} = \arg\min_{f} \frac{1}{2}\|y - f\|_2^2 + \lambda_1 \|A_{\mathrm{LPL}} f\|_1 + \frac{\lambda_2}{2}\|C_{\mathrm{sync}} f\|_2^2.$$

Usage

```
fit.slpl.tf(
  X = NULL,
  y,
  operator = NULL,
  lambda1 = NULL,
  lambda2 = 0,
  lambda1.grid = NULL,
  lambda2.grid = NULL,
  lambda.selection = c("fixed", "cv"),
  operator.grid = NULL,
  foldid = NULL,
```

```
  cv.folds = 5L,
  cv.loss = c("mse", "rmse", "mae"),
  cv.seed = NULL,
  cv.repeats = 1L,
  solver = c("genlasso"),
  selection = c("min", "one.se"),
  maxsteps = 2000L,
  minlam = 0,
  approx = FALSE,
  rtol = 1e-07,
  btol = 1e-07,
  eps = 1e-04,
  verbose = FALSE,
  ...
)
```

Arguments

`X`	Optional coordinate matrix used to build `slpl.tf.operator` when `operator` is `NULL`.
`y`	Numeric response vector.
`operator`	Optional `"slpl_tf_operator"` object.
`lambda1`	Fixed LPL-TF ℓ_1 penalty, or a shortcut for `lambda1.grid` when `lambda.selection = "cv"`.
`lambda2`	Fixed quadratic synchronization penalty, or a shortcut for `lambda2.grid` when `lambda.selection = "cv"`.
`lambda1.grid`	Optional nonnegative λ_1 grid for CV.
`lambda2.grid`	Optional nonnegative λ_2 grid for CV.
`lambda.selection`	`"fixed"` or `"cv"`. CV uses materialized folds and a deterministic Cartesian grid over `lambda1.grid` and `lambda2.grid`.
`operator.grid`	Optional Phase-S3 operator candidate grid. Supply a data frame with one row per candidate or a list of named lists.
`foldid`	Optional deterministic fold assignments for CV.
`cv.folds`	Number of generated folds when `foldid = NULL`.
`cv.loss`	Cross-validation loss, `"mse"`, `"rmse"`, or `"mae"`.
`cv.seed`	Optional seed for reproducible generated folds.
`cv.repeats`	Phase S3 supports only one CV repeat.
`solver`	Current implementation supports only `"genlasso"`.
`selection`	Selection rule, `"min"` or `"one.se"`. For the two-parameter one-standard-error rule, the most regularized eligible pair is chosen by decreasing `lambda1` and then decreasing `lambda2`.
`maxsteps`, `minlam`, `approx`, `rtol`, `btol`, `eps`	Genlasso controls.

verbose	Logical.
...	Additional arguments passed to slpl.tf.operator when the operator is built internally.

Value

A list of class "slpl_tf".

Examples

```
if (requireNamespace("genlasso", quietly = TRUE)) {
  X <- matrix(seq(0, 1, length.out = 18), ncol = 1)
  fit.slpl.tf(X, sin(2 * pi * X[, 1]), degree = 1L,
              support.type = "knn", support.size = 7L,
              lambda1 = 0.1, lambda2 = 0, lambda.selection = "fixed")
}
```

---

fit.ssrhe.hessian.l1.regression

Fit SSRHE-Style Hessian L1 Regression

Description

Fits an ℓ_1-adaptive SSRHE Hessian comparator using the row operator A from ssrhe.hessian.operator:

$$\widehat{f}_\lambda = \arg\min_f \left\{ \frac{1}{2} \sum_i w_i (y_i - f_i)^2 + \lambda \|Af\|_1 \right\}.$$

Usage

```
fit.ssrhe.hessian.l1.regression(
  X,
  y,
  k = NULL,
  tangent.dim,
  lambda.grid = NULL,
  lambda.selection = c("cv", "fixed"),
  weights = NULL,
  n.lambda = 40L,
  nfolds = 5L,
  fold.id = NULL,
  loss = c("mse", "mae"),
  selection = c("min", "one.se"),
  nn.index = NULL,
  neighborhood.type = c("knn", "adaptive.radius", "supplied"),
  support.index = NULL,
  adaptive.k.scale = NULL,
```

```
  radius.rule = c("geomean", "max", "min"),
  radius.factor = 1.25,
  min.support = NULL,
  max.support = NULL,
  support.buffer = 2L,
  support.topup = c("nearest", "none"),
  tangent.dim.rule = c("fixed", "eigen.cumulative"),
  eigen.tolerance = 0.95,
  derivative.order = 2L,
  pinv.tol = sqrt(.Machine$double.eps),
  local.solver = c("auto", "normal.equations", "svd", "qr"),
  normal.equations.max.condition = 10000,
  solver = c("genlasso", "admm", "auto"),
  row.scaling = c("none", "l2"),
  admm.rho = 1,
  admm.maxiter = 2000L,
  admm.abstol = 1e-04,
  admm.reltol = 0.001,
  maxsteps = 2000L,
  minlam = 0,
  approx = FALSE,
  rtol = 1e-07,
  btol = 1e-07,
  eps = 1e-04,
  support.selection = c("rule", "cv"),
  support.grid = NULL,
  support.cv.max.candidates = 8L,
  return.local.diagnostics = FALSE,
  return.timing = FALSE,
  verbose = FALSE
)
```

Arguments

X	Numeric matrix with one observation per row. Distances for the default neighborhood search are Euclidean distances in these coordinates.
y	Numeric response vector of length nrow(X). Matrix responses are not yet supported for the ℓ_1 path.
k	Integer number of nearest neighbors per point, including the point itself, used when neighborhood.type = "knn". This follows the SSRHE Matlab convention. For adaptive-radius neighborhoods, k may be omitted when adaptive.k.scale is supplied.
tangent.dim	Integer tangent dimension used for the local PCA chart. Required when tangent.dim.rule = "fixed". If NULL and tangent.dim.rule = "eigen.cumulative", the dimension is selected locally from the PCA variance ratio.
lambda.grid	Optional nonnegative lambda grid. For lambda.selection = "fixed", this must contain exactly one value. For lambda.selection = "cv", NULL builds a default grid from the fitted full-data generalized-lasso path.

`lambda.selection`
: `"cv"` for observed-label K-fold cross-validation or `"fixed"` for a supplied fixed lambda.

`weights`
: Optional nonnegative observation weights. Missing responses automatically receive zero weight.

`n.lambda`
: Number of default lambda candidates when `lambda.grid = NULL` and `lambda.selection = "cv"`.

`nfolds`
: Number of validation folds over observed positive-weight labels. Ignored when `fold.id` is supplied.

`fold.id`
: Optional integer fold assignments of length `nrow(X)`.

`loss`
: Validation loss, currently `"mse"` or `"mae"`.

`selection`
: Selection rule. `"min"` chooses the smallest mean validation loss. `"one.se"` chooses the largest lambda within one standard error of the minimum.

`nn.index`
: Optional integer matrix of neighbor indices, with `nrow(X)` rows and `k` columns. Each row must contain its center vertex. If `NULL`, Euclidean k-NN including self is computed in C++.

`neighborhood.type`
: Local support rule. `"knn"` uses the original rectangular self-including kNN neighborhoods. `"adaptive.radius"` builds variable-size supports from `dgraphs::create.rknn.graph` `"supplied"` uses `support.index` directly.

`support.index`
: Optional list of integer vectors, one per row of `X`. Each element gives a variable-size local support and must contain its center vertex.

`adaptive.k.scale`
: Integer local-scale k used by `dgraphs::create.rknn.graph()` when `neighborhood.type = "adaptive.radius"`.

`radius.rule`, `radius.factor`
: Adaptive-radius graph parameters passed to `dgraphs::create.rknn.graph()`.

`min.support`
: Optional minimum local support size for adaptive-radius supports. Defaults to the local quadratic design size plus `support.buffer`, clamped to `nrow(X)`.

`max.support`
: Optional maximum local support size. Oversized adaptive supports are trimmed to the closest `max.support` vertices while keeping the center vertex.

`support.buffer`
: Nonnegative integer added to the local quadratic design size when choosing the default `min.support`.

`support.topup`
: How undersized adaptive-radius supports are enlarged. `"nearest"` appends ambient nearest neighbors. `"none"` leaves supports unchanged and lets the C++ operator reject undersized supports.

`tangent.dim.rule`
: Either `"fixed"` or `"eigen.cumulative"`.

`eigen.tolerance`
: Cumulative local PCA variance threshold used when `tangent.dim.rule = "eigen.cumulative"` and `tangent.dim = NULL`.

`derivative.order`
: Integer derivative order of the local SSRHE-style operator. `2L` is the original local Hessian energy. `3L` is an experimental third-derivative energy whose rows estimate unique symmetric third-derivative tensor components with factorial and tensor-multiplicity scaling.

`pinv.tol` Nonnegative tolerance multiplier for local pseudoinverses.

`local.solver` Local least-squares backend used to map local function values to derivative coefficients. `"auto"` is the default: it uses normal equations when the local design is full rank and has condition number no larger than `normal.equations.max.condition`, and otherwise falls back to SVD. `"normal.equations"` requests the normal-equation solve for full-rank local designs and falls back only on hard numerical failures. `"svd"` is the most stable reference path. `"qr"` uses pivoted QR and falls back to SVD for rank-deficient local designs.

`normal.equations.max.condition`
Positive condition-number guard used by `local.solver = "auto"` before accepting the normal-equation backend. The default is deliberately conservative because normal-equation solves square the effective condition number and order-3 near-minimum local supports can be numerically fragile.

`solver` Solver backend. `"genlasso"` uses the generalized-lasso path backend. `"admm"` uses a fixed-lambda ADMM solver for each lambda value. `"auto"` tries `"genlasso"` first and falls back to ADMM when path extraction produces an error or non-finite fitted values.

`row.scaling` Optional row scaling for the penalty matrix before solving. `"l2"` scales nonzero rows of A to unit Euclidean norm.

`admm.rho`, `admm.maxiter`, `admm.abstol`, `admm.reltol`
ADMM controls used when `solver = "admm"` or when `solver = "auto"` falls back to ADMM.

`maxsteps`, `minlam`, `approx`, `rtol`, `btol`, `eps`, `verbose`
Controls passed to **genlasso**.

`support.selection`
Support-profile selection rule. `"rule"` uses the supplied `adaptive.k.scale`, `min.support`, and `max.support`. `"cv"` is currently supported for `neighborhood.type = "adaptive.radius"` with `lambda.selection = "cv"` and chooses among rows of `support.grid` by an outer response cross-validation loop.

`support.grid` Optional data frame of support profiles with columns `adaptive.k.scale`, `min.support`, and optional `max.support`. If `NULL`, `ssrhe.support.grid` builds a compact default grid.

`support.cv.max.candidates`
Maximum number of support profiles to try when `support.selection = "cv"`.

`return.local.diagnostics`
Logical. If `TRUE`, compute additional R-side local chart diagnostics such as chart distortion and boundary asymmetry. These diagnostics are useful for operator audits, but can be skipped in fitting and cross-validation paths for speed.

`return.timing` Logical. If `TRUE`, attach a phase-level elapsed time table to the returned operator. The timings separate R-side validation, neighborhood/support construction, native local operator construction, optional local diagnostics, sparse matrix assembly, and output finalization. For adaptive-radius neighborhoods, subphase timings are also attached in `neighborhoods$timing`.

Details

This function exposes the SSRHE local polynomial derivative estimator as an ℓ_1 penalty, rather than as the original SSRHE ℓ_2 Hessian-energy penalty used by `fit.ssrhe.hessian.regression`. With

`derivative.order = 2L`, A contains local quadratic/Hessian rows. With `derivative.order = 3L`, A contains local cubic third-derivative tensor rows with the same symmetric component scaling used by `ssrhe.hessian.operator`. The existing ℓ_2 fit solves a linear system involving $B = A^\top A$. This function instead keeps the rows of A and penalizes their absolute values. It is therefore closer in spirit to graph trend filtering, while retaining SSRHE's local-PCA derivative construction.

The default solver backend is **genlasso**. For larger or numerically fragile third-order operators, `solver = "admm"` fits the requested lambda values directly without computing a generalized-lasso path, and `solver = "auto"` falls back to ADMM when the path backend fails or returns non-finite fitted values. Cross-validation removes held-out labels from the data-fit term by setting their weights to zero, then scores predictions on those held-out labels.

With `support.selection = "cv"`, each adaptive-radius support candidate builds a fresh SSRHE operator and runs the usual lambda CV with shared fold assignments. The selected fit is the candidate with the smallest selected CV error. This is useful when the default support-size rule is too rigid, but it can be much slower than tuning lambda for one fixed operator.

Value

A list of class `"ssrhe.hessian.l1.fit"` containing fitted values, residuals, selected lambda, the SSRHE operator, generalized-lasso path metadata, lambda-grid fitted values, and CV diagnostics when requested.

References

Kim, K. I., Steinke, F., and Hein, M. (2009). Semi-supervised regression using Hessian energy with an application to semi-supervised dimensionality reduction. *Advances in Neural Information Processing Systems 22*. https://papers.nips.cc/paper_files/paper/2009/hash/f4552671f8909587cf485ea990207f3b-Abstract.html

Examples

```
X <- matrix(seq(0, 1, length.out = 12), ncol = 1)
fit.ssrhe.hessian.l1.regression(
  X, sin(2 * pi * X[, 1]), k = 6L, tangent.dim = 1L,
  lambda.grid = 0.05, lambda.selection = "fixed", solver = "admm"
)
```

---

fit.ssrhe.hessian.regression

Fit SSRHE-Style Hessian-Energy Regression

Description

Fits the ℓ_2 Hessian-energy regularized estimator associated with `ssrhe.hessian.operator`. This is a direct SSRHE-style comparator for Hessian smoothing on point clouds; it is not a replacement for graph trend-filtering regression and is distinct from ℓ_1-adaptive graph trend filtering.

Usage

```
fit.ssrhe.hessian.regression(
  X,
  y,
  k = NULL,
  tangent.dim,
  lambda1,
  lambda2 = 0,
  weights = NULL,
  nn.index = NULL,
  neighborhood.type = c("knn", "adaptive.radius", "supplied"),
  support.index = NULL,
  adaptive.k.scale = NULL,
  radius.rule = c("geomean", "max", "min"),
  radius.factor = 1.25,
  min.support = NULL,
  max.support = NULL,
  support.buffer = 2L,
  support.topup = c("nearest", "none"),
  tangent.dim.rule = c("fixed", "eigen.cumulative"),
  eigen.tolerance = 0.95,
  derivative.order = 2L,
  stabilizer = lambda2 > 0,
  pinv.tol = sqrt(.Machine$double.eps),
  local.solver = c("auto", "normal.equations", "svd", "qr"),
  normal.equations.max.condition = 10000,
  ridge = 0,
  return.A = TRUE,
  return.local.diagnostics = FALSE,
  return.timing = FALSE,
  verbose = FALSE
)
```

Arguments

X	Numeric matrix with one observation per row. Distances for the default neighborhood search are Euclidean distances in these coordinates.
y	Numeric response vector of length nrow(X) or numeric matrix with nrow(X) rows. Matrix columns are fit as separate responses. NA values are allowed and are treated as unobserved by setting the corresponding observation weight to zero.
k	Integer number of nearest neighbors per point, including the point itself, used when neighborhood.type = "knn". This follows the SSRHE Matlab convention. For adaptive-radius neighborhoods, k may be omitted when adaptive.k.scale is supplied.
tangent.dim	Integer tangent dimension used for the local PCA chart. Required when tangent.dim.rule = "fixed". If NULL and tangent.dim.rule = "eigen.cumulative", the dimension is selected locally from the PCA variance ratio.

`lambda1` Nonnegative Hessian-energy penalty multiplier for $f^\top Bf = \|Af\|_2^2$.

`lambda2` Nonnegative supplemental-stabilizer multiplier for $f^\top B_S f$. If positive, `stabilizer` must be `TRUE`. Currently supported only for `derivative.order = 2L`.

`weights` Optional nonnegative observation weights. May be `NULL`, a vector of length `nrow(X)`, or a matrix with the same dimensions as `y`.

`nn.index` Optional integer matrix of neighbor indices, with `nrow(X)` rows and `k` columns. Each row must contain its center vertex. If `NULL`, Euclidean k-NN including self is computed in C++.

`neighborhood.type`
Local support rule. `"knn"` uses the original rectangular self-including kNN neighborhoods. `"adaptive.radius"` builds variable-size supports from `dgraphs::create.rknn.graph` `"supplied"` uses `support.index` directly.

`support.index` Optional list of integer vectors, one per row of `X`. Each element gives a variable-size local support and must contain its center vertex.

`adaptive.k.scale`
Integer local-scale k used by `dgraphs::create.rknn.graph()` when `neighborhood.type = "adaptive.radius"`.

`radius.rule`, `radius.factor`
Adaptive-radius graph parameters passed to `dgraphs::create.rknn.graph()`.

`min.support` Optional minimum local support size for adaptive-radius supports. Defaults to the local quadratic design size plus `support.buffer`, clamped to `nrow(X)`.

`max.support` Optional maximum local support size. Oversized adaptive supports are trimmed to the closest `max.support` vertices while keeping the center vertex.

`support.buffer` Nonnegative integer added to the local quadratic design size when choosing the default `min.support`.

`support.topup` How undersized adaptive-radius supports are enlarged. `"nearest"` appends ambient nearest neighbors. `"none"` leaves supports unchanged and lets the C++ operator reject undersized supports.

`tangent.dim.rule`
Either `"fixed"` or `"eigen.cumulative"`.

`eigen.tolerance`
Cumulative local PCA variance threshold used when `tangent.dim.rule = "eigen.cumulative"` and `tangent.dim = NULL`.

`derivative.order`
Integer derivative order of the local SSRHE-style operator. `2L` is the original local Hessian energy. `3L` is an experimental third-derivative energy whose rows estimate unique symmetric third-derivative tensor components with factorial and tensor-multiplicity scaling.

`stabilizer` Logical. If `TRUE`, also construct the supplemental stabilizer matrix described in the SSRHE supplement. Currently supported only for `derivative.order = 2L`.

`pinv.tol` Nonnegative tolerance multiplier for local pseudoinverses.

`local.solver` Local least-squares backend used to map local function values to derivative coefficients. `"auto"` is the default: it uses normal equations when the local design is full rank and has condition number no larger than `normal.equations.max.condition`,

and otherwise falls back to SVD. "normal.equations" requests the normal-equation solve for full-rank local designs and falls back only on hard numerical failures. "svd" is the most stable reference path. "qr" uses pivoted QR and falls back to SVD for rank-deficient local designs.

normal.equations.max.condition
: Positive condition-number guard used by local.solver = "auto" before accepting the normal-equation backend. The default is deliberately conservative because normal-equation solves square the effective condition number and order-3 near-minimum local supports can be numerically fragile.

ridge
: Nonnegative diagonal ridge added to the linear system for numerical stabilization.

return.A
: Logical. If TRUE, return A as a sparse matrix.

return.local.diagnostics
: Logical. If TRUE, compute additional R-side local chart diagnostics such as chart distortion and boundary asymmetry. These diagnostics are useful for operator audits, but can be skipped in fitting and cross-validation paths for speed.

return.timing
: Logical. If TRUE, attach a phase-level elapsed time table to the returned operator. The timings separate R-side validation, neighborhood/support construction, native local operator construction, optional local diagnostics, sparse matrix assembly, and output finalization. For adaptive-radius neighborhoods, subphase timings are also attached in neighborhoods$timing.

verbose
: Logical. If TRUE, print a short native construction message.

Details

For each response column, this function solves

$$(W + \lambda_1 B + \lambda_2 B_S + \epsilon I)\hat{f} = Wy,$$

where W is the diagonal matrix of observation weights and ϵ is ridge. Fully observed data with lambda1 = lambda2 = ridge = 0 therefore reproduce the observed response exactly. Missing responses are excluded from the data-fit term by setting their weights to zero. The Matlab SSRHE semi-supervised convention is represented by a 0/1 labeled-indicator weights vector, or equivalently by setting unlabeled responses to NA: labeled vertices contribute unit diagonal data-fit terms and unlabeled vertices contribute no data-fit term.

The lower-level operator is matched to the Kim–Steinke–Hein SSRHE Matlab construction: self-including kNN neighborhoods, local PCA charts, a fixed-intercept local quadratic fit, doubled diagonal Hessian components, and optional supplemental stabilizer. The package exposes both A and $B = A^\top A$; the fitted ℓ_2 estimator uses B.

Value

A list of class "ssrhe.hessian.fit" containing fitted values, residuals, input response, weights, lambda parameters, objective/energy diagnostics, the reused operator, solver metadata, and the call.

References

Kim, K. I., Steinke, F., and Hein, M. (2009). Semi-supervised regression using Hessian energy with an application to semi-supervised dimensionality reduction. *Advances in Neural Information Processing Systems 22*. https://papers.nips.cc/paper_files/paper/2009/hash/f4552671f8909587cf485ea990207f3b-Abstract.html

Examples

```
X <- matrix(seq(0, 1, length.out = 12), ncol = 1)
fit.ssrhe.hessian.regression(
  X, sin(2 * pi * X[, 1]), k = 6L, tangent.dim = 1L, lambda1 = 0.1
)
```

---

fit.ssrhe.hessian.regression.cv

Select SSRHE Hessian Regression Penalties by Label Cross-Validation

---

Description

Fits `fit.ssrhe.hessian.regression` over a grid of fixed `lambda1`/`lambda2` values using cross-validation on observed labels. This is intended for semi-supervised SSRHE use: validation folds are formed only from entries that are observed and have positive data-fit weight.

Usage

```
fit.ssrhe.hessian.regression.cv(
  X,
  y,
  k = NULL,
  tangent.dim,
  lambda1.grid,
  lambda2.grid = 0,
  weights = NULL,
  nfolds = 5L,
  fold.id = NULL,
  loss = c("mse", "mae"),
  selection = c("min", "one.se"),
  nn.index = NULL,
  neighborhood.type = c("knn", "adaptive.radius", "supplied"),
  support.index = NULL,
  adaptive.k.scale = NULL,
  radius.rule = c("geomean", "max", "min"),
  radius.factor = 1.25,
  min.support = NULL,
  max.support = NULL,
  support.buffer = 2L,
  support.topup = c("nearest", "none"),
```

```
  tangent.dim.rule = c("fixed", "eigen.cumulative"),
  eigen.tolerance = 0.95,
  derivative.order = 2L,
  stabilizer = any(lambda2.grid > 0),
  pinv.tol = sqrt(.Machine$double.eps),
  local.solver = c("auto", "normal.equations", "svd", "qr"),
  normal.equations.max.condition = 10000,
  ridge = 0,
  return.A = TRUE,
  return.local.diagnostics = FALSE,
  return.timing = FALSE,
  support.selection = c("rule", "cv"),
  support.grid = NULL,
  support.cv.max.candidates = 8L,
  verbose = FALSE
)
```

Arguments

X	Numeric matrix with one observation per row. Distances for the default neighborhood search are Euclidean distances in these coordinates.
y	Numeric response vector of length nrow(X) or numeric matrix with nrow(X) rows. Matrix columns are fit as separate responses. NA values are allowed and are treated as unobserved by setting the corresponding observation weight to zero.
k	Integer number of nearest neighbors per point, including the point itself, used when neighborhood.type = "knn". This follows the SSRHE Matlab convention. For adaptive-radius neighborhoods, k may be omitted when adaptive.k.scale is supplied.
tangent.dim	Integer tangent dimension used for the local PCA chart. Required when tangent.dim.rule = "fixed". If NULL and tangent.dim.rule = "eigen.cumulative", the dimension is selected locally from the PCA variance ratio.
lambda1.grid	Nonnegative numeric vector of Hessian-energy penalty candidates.
lambda2.grid	Nonnegative numeric vector of supplemental-stabilizer penalty candidates. Use 0 to omit the supplemental stabilizer from selection.
weights	Optional nonnegative observation weights. May be NULL, a vector of length nrow(X), or a matrix with the same dimensions as y.
nfolds	Number of validation folds over observed positive-weight labels. Ignored when fold.id is supplied.
fold.id	Optional integer vector of length nrow(X) assigning observed positive-weight labels to validation folds. Nonpositive or NA entries are ignored.
loss	Validation loss, currently "mse" or "mae".
selection	Selection rule. "min" chooses the smallest mean validation loss. "one.se" chooses the largest total penalty among candidates within one standard error of the minimum.

`nn.index` Optional integer matrix of neighbor indices, with `nrow(X)` rows and `k` columns. Each row must contain its center vertex. If `NULL`, Euclidean k-NN including self is computed in C++.

`neighborhood.type` Local support rule. `"knn"` uses the original rectangular self-including kNN neighborhoods. `"adaptive.radius"` builds variable-size supports from `dgraphs::create.rknn.graph`. `"supplied"` uses `support.index` directly.

`support.index` Optional list of integer vectors, one per row of `X`. Each element gives a variable-size local support and must contain its center vertex.

`adaptive.k.scale` Integer local-scale k used by `dgraphs::create.rknn.graph()` when `neighborhood.type = "adaptive.radius"`.

`radius.rule`, `radius.factor` Adaptive-radius graph parameters passed to `dgraphs::create.rknn.graph()`.

`min.support` Optional minimum local support size for adaptive-radius supports. Defaults to the local quadratic design size plus `support.buffer`, clamped to `nrow(X)`.

`max.support` Optional maximum local support size. Oversized adaptive supports are trimmed to the closest `max.support` vertices while keeping the center vertex.

`support.buffer` Nonnegative integer added to the local quadratic design size when choosing the default `min.support`.

`support.topup` How undersized adaptive-radius supports are enlarged. `"nearest"` appends ambient nearest neighbors. `"none"` leaves supports unchanged and lets the C++ operator reject undersized supports.

`tangent.dim.rule` Either `"fixed"` or `"eigen.cumulative"`.

`eigen.tolerance` Cumulative local PCA variance threshold used when `tangent.dim.rule = "eigen.cumulative"` and `tangent.dim = NULL`.

`derivative.order` Integer derivative order of the local SSRHE-style operator. `2L` is the original local Hessian energy. `3L` is an experimental third-derivative energy whose rows estimate unique symmetric third-derivative tensor components with factorial and tensor-multiplicity scaling.

`stabilizer` Logical. If `TRUE`, also construct the supplemental stabilizer matrix described in the SSRHE supplement. Currently supported only for `derivative.order = 2L`.

`pinv.tol` Nonnegative tolerance multiplier for local pseudoinverses.

`local.solver` Local least-squares backend used to map local function values to derivative coefficients. `"auto"` is the default: it uses normal equations when the local design is full rank and has condition number no larger than `normal.equations.max.condition`, and otherwise falls back to SVD. `"normal.equations"` requests the normal-equation solve for full-rank local designs and falls back only on hard numerical failures. `"svd"` is the most stable reference path. `"qr"` uses pivoted QR and falls back to SVD for rank-deficient local designs.

`normal.equations.max.condition`
: Positive condition-number guard used by `local.solver = "auto"` before accepting the normal-equation backend. The default is deliberately conservative because normal-equation solves square the effective condition number and order-3 near-minimum local supports can be numerically fragile.

`ridge`
: Nonnegative diagonal ridge added to the linear system for numerical stabilization.

`return.A`
: Logical. If `TRUE`, return A as a sparse matrix.

`return.local.diagnostics`
: Logical. If `TRUE`, compute additional R-side local chart diagnostics such as chart distortion and boundary asymmetry. These diagnostics are useful for operator audits, but can be skipped in fitting and cross-validation paths for speed.

`return.timing`
: Logical. If `TRUE`, attach a phase-level elapsed time table to the returned operator. The timings separate R-side validation, neighborhood/support construction, native local operator construction, optional local diagnostics, sparse matrix assembly, and output finalization. For adaptive-radius neighborhoods, subphase timings are also attached in `neighborhoods$timing`.

`support.selection`
: Support-profile selection rule. `"rule"` uses the supplied `adaptive.k.scale`, `min.support`, and `max.support`. `"cv"` is currently supported for `neighborhood.type = "adaptive.radius"` and chooses among rows of `support.grid` by outer response cross-validation.

`support.grid`
: Optional data frame of support profiles with columns `adaptive.k.scale`, `min.support`, and optional `max.support`. If `NULL`, `ssrhe.support.grid` builds a compact default grid.

`support.cv.max.candidates`
: Maximum number of support profiles to try when `support.selection = "cv"`.

`verbose`
: Logical. If `TRUE`, print a short native construction message.

Details

For each validation fold, the held-out labels are removed from the data-fit term by setting their weights to zero. The fitted values are then scored only on those held-out labels. The final returned fit is refit with the selected penalties using all observed positive-weight labels.

With `support.selection = "cv"`, this function performs an outer support-profile selection loop. For each candidate adaptive-radius support profile, it constructs a fresh SSRHE operator, runs the usual `lambda1.grid`/`lambda2.grid` cross-validation with the same fold assignments, and selects the support profile with the smallest selected CV error. This can substantially increase runtime because local operator construction and lambda CV are nested.

The current implementation supports a single response vector. Matrix-response penalty selection should be performed column-by-column.

Value

A list of class `"ssrhe.hessian.cv.fit"` and `"ssrhe.hessian.fit"` containing the final fit plus `cv.table`, `fold.id`, and `selection` diagnostics.

Examples

```
X <- matrix(seq(0, 1, length.out = 12), ncol = 1)
fit.ssrhe.hessian.regression.cv(
  X, sin(2 * pi * X[, 1]), k = 6L, tangent.dim = 1L,
  lambda1.grid = c(0.01, 0.1), nfolds = 2L
)
```

`fit.ssrhe.hessian.regression.gcv`
Select SSRHE Hessian Regression Penalties by GCV

Description

Fits `fit.ssrhe.hessian.regression` over a grid of `lambda1`/`lambda2` values and selects penalties by generalized cross-validation (GCV). This is a faster, deterministic alternative to label-fold CV for fully observed SSRHE ℓ_2 smoothing problems. The smoother trace can be computed exactly, or estimated by a Hutchinson randomized trace estimator for larger grids.

Usage

```
fit.ssrhe.hessian.regression.gcv(
  X,
  y,
  k = NULL,
  tangent.dim,
  lambda1.grid,
  lambda2.grid = 0,
  weights = NULL,
  nn.index = NULL,
  neighborhood.type = c("knn", "adaptive.radius", "supplied"),
  support.index = NULL,
  adaptive.k.scale = NULL,
  radius.rule = c("geomean", "max", "min"),
  radius.factor = 1.25,
  min.support = NULL,
  max.support = NULL,
  support.buffer = 2L,
  support.topup = c("nearest", "none"),
  tangent.dim.rule = c("fixed", "eigen.cumulative"),
  eigen.tolerance = 0.95,
  derivative.order = 2L,
  stabilizer = any(lambda2.grid > 0),
  pinv.tol = sqrt(.Machine$double.eps),
  local.solver = c("auto", "normal.equations", "svd", "qr"),
  normal.equations.max.condition = 10000,
  ridge = 0,
  return.A = TRUE,
```

```
  return.local.diagnostics = FALSE,
  return.timing = FALSE,
  support.selection = c("rule", "gcv"),
  support.grid = NULL,
  support.gcv.max.candidates = 8L,
  gcv.trace.method = c("exact", "hutchinson"),
  gcv.trace.n.probes = 50L,
  gcv.trace.seed = NULL,
  verbose = FALSE
)
```

Arguments

X	Numeric matrix with one observation per row. Distances for the default neighborhood search are Euclidean distances in these coordinates.
y	Numeric response vector of length nrow(X) or numeric matrix with nrow(X) rows. Matrix columns are fit as separate responses. NA values are allowed and are treated as unobserved by setting the corresponding observation weight to zero.
k	Integer number of nearest neighbors per point, including the point itself, used when neighborhood.type = "knn". This follows the SSRHE Matlab convention. For adaptive-radius neighborhoods, k may be omitted when adaptive.k.scale is supplied.
tangent.dim	Integer tangent dimension used for the local PCA chart. Required when tangent.dim.rule = "fixed". If NULL and tangent.dim.rule = "eigen.cumulative", the dimension is selected locally from the PCA variance ratio.
lambda1.grid	Nonnegative numeric vector of Hessian-energy penalty candidates.
lambda2.grid	Nonnegative numeric vector of supplemental-stabilizer penalty candidates. Use 0 to omit the supplemental stabilizer from selection.
weights	Optional nonnegative observation weights. May be NULL, a vector of length nrow(X), or a matrix with the same dimensions as y.
nn.index	Optional integer matrix of neighbor indices, with nrow(X) rows and k columns. Each row must contain its center vertex. If NULL, Euclidean k-NN including self is computed in C++.
neighborhood.type	Local support rule. "knn" uses the original rectangular self-including kNN neighborhoods. "adaptive.radius" builds variable-size supports from dgraphs::create.rknn.graph "supplied" uses support.index directly.
support.index	Optional list of integer vectors, one per row of X. Each element gives a variable-size local support and must contain its center vertex.
adaptive.k.scale	Integer local-scale k used by dgraphs::create.rknn.graph() when neighborhood.type = "adaptive.radius".
radius.rule, radius.factor	Adaptive-radius graph parameters passed to dgraphs::create.rknn.graph().

`min.support` Optional minimum local support size for adaptive-radius supports. Defaults to the local quadratic design size plus `support.buffer`, clamped to `nrow(X)`.

`max.support` Optional maximum local support size. Oversized adaptive supports are trimmed to the closest `max.support` vertices while keeping the center vertex.

`support.buffer` Nonnegative integer added to the local quadratic design size when choosing the default `min.support`.

`support.topup` How undersized adaptive-radius supports are enlarged. `"nearest"` appends ambient nearest neighbors. `"none"` leaves supports unchanged and lets the C++ operator reject undersized supports.

`tangent.dim.rule`
Either `"fixed"` or `"eigen.cumulative"`.

`eigen.tolerance`
Cumulative local PCA variance threshold used when `tangent.dim.rule = "eigen.cumulative"` and `tangent.dim = NULL`.

`derivative.order`
Integer derivative order of the local SSRHE-style operator. `2L` is the original local Hessian energy. `3L` is an experimental third-derivative energy whose rows estimate unique symmetric third-derivative tensor components with factorial and tensor-multiplicity scaling.

`stabilizer` Logical. If `TRUE`, also construct the supplemental stabilizer matrix described in the SSRHE supplement. Currently supported only for `derivative.order = 2L`.

`pinv.tol` Nonnegative tolerance multiplier for local pseudoinverses.

`local.solver` Local least-squares backend used to map local function values to derivative coefficients. `"auto"` is the default: it uses normal equations when the local design is full rank and has condition number no larger than `normal.equations.max.condition`, and otherwise falls back to SVD. `"normal.equations"` requests the normal-equation solve for full-rank local designs and falls back only on hard numerical failures. `"svd"` is the most stable reference path. `"qr"` uses pivoted QR and falls back to SVD for rank-deficient local designs.

`normal.equations.max.condition`
Positive condition-number guard used by `local.solver = "auto"` before accepting the normal-equation backend. The default is deliberately conservative because normal-equation solves square the effective condition number and order-3 near-minimum local supports can be numerically fragile.

`ridge` Nonnegative diagonal ridge added to the linear system for numerical stabilization.

`return.A` Logical. If `TRUE`, return A as a sparse matrix.

`return.local.diagnostics`
Logical. If `TRUE`, compute additional R-side local chart diagnostics such as chart distortion and boundary asymmetry. These diagnostics are useful for operator audits, but can be skipped in fitting and cross-validation paths for speed.

`return.timing` Logical. If `TRUE`, attach a phase-level elapsed time table to the returned operator. The timings separate R-side validation, neighborhood/support construction, native local operator construction, optional local diagnostics, sparse matrix assembly, and output finalization. For adaptive-radius neighborhoods, subphase timings are also attached in `neighborhoods$timing`.

`support.selection`
: Support-profile selection rule. `"rule"` uses the supplied `adaptive.k.scale`, `min.support`, and `max.support`. `"gcv"` is currently supported for `neighborhood.type = "adaptive.radius"` and chooses among rows of `support.grid` by outer GCV.

`support.grid`
: Optional data frame of support profiles with columns `adaptive.k.scale`, `min.support`, and optional `max.support`. If `NULL`, `ssrhe.support.grid` builds a compact default grid.

`support.gcv.max.candidates`
: Maximum number of support profiles to try when `support.selection = "gcv"`.

`gcv.trace.method`
: Method used to compute the smoother trace in the GCV score. `"exact"` solves against the full diagonal weight matrix. `"hutchinson"` estimates the trace with Rademacher probe vectors.

`gcv.trace.n.probes`
: Number of Hutchinson probe vectors to use when `gcv.trace.method = "hutchinson"`.

`gcv.trace.seed`
: Optional integer seed for reproducible Hutchinson trace estimates.

`verbose`
: Logical. If `TRUE`, print a short native construction message.

Details

For a fixed SSRHE operator, the ℓ_2 fit is a linear smoother

$$\hat{f}_\lambda = S_\lambda y, \qquad S_\lambda = (W + \lambda_1 B + \lambda_2 B_S + \epsilon I)^{-1} W,$$

where W is the diagonal observation-weight matrix and ϵ is `ridge`. By default this function computes the exact smoother trace $\mathrm{tr}(S_\lambda)$ and scores each grid point by

$$\mathrm{GCV}(\lambda) = \frac{n^{-1} \sum_i w_i (y_i - \hat{f}_i)^2}{(1 - \mathrm{tr}(S_\lambda)/n)^2}.$$

With `gcv.trace.method = "hutchinson"`, the trace is estimated by

$$\mathrm{tr}(S_\lambda) = \mathbb{E}\{z^\top S_\lambda z\},$$

using independent Rademacher vectors z. Each probe requires one solve with right-hand side Wz. The estimate is stochastic but can be made reproducible with `gcv.trace.seed`; the returned GCV table reports the trace standard error.

The current implementation requires a single fully observed response vector and strictly positive observation weights. Semi-supervised or missing-label SSRHE tuning should continue to use `fit.ssrhe.hessian.regression.cv`.

With `support.selection = "gcv"`, this function performs an outer adaptive-radius support-profile loop. Each support candidate constructs a fresh SSRHE operator, runs the same exact GCV grid search, and the candidate with the smallest selected GCV is refit and returned.

Value

A list of class `"ssrhe.hessian.gcv.fit"` and `"ssrhe.hessian.fit"` containing the final fit plus `gcv.table`, `selection`, and optional `support.gcv.table` diagnostics.

Examples

```
X <- matrix(seq(0, 1, length.out = 12), ncol = 1)
fit.ssrhe.hessian.regression.gcv(
  X, sin(2 * pi * X[, 1]), k = 6L, tangent.dim = 1L,
  lambda1.grid = c(0.01, 0.1)
)
```

`fit.subject.od` *Fit Subject-Occupation Density*

Description

Convenience wrapper that converts subject visit indices into a density input. Density-native methods dispatch to `fit.density`. LPS/PS-LPS methods fit ordinary smoother objects first and then call `normalize.density`; they are subject-occupation workflows, not standalone density-native methods.

Usage

```
fit.subject.od(
  X,
  subject.index,
  method = c("empirical", "graph_random_walk", "lps_count", "ps_lps_count",
    "lps_logistic_binary", "chart_kernel", "local_likelihood_density",
    "local_likelihood_bernoulli"),
  graph = NULL,
  graph.control = list(),
  od.control = list(),
  return.details = TRUE,
  od.cv = c("none", "visit"),
  visit.foldid = NULL,
  visit.cv.folds = 5L,
  visit.cv.seed = 1L,
  visit.cv.epsilon = 1e-15,
  ...
)
```

Arguments

`X`	Numeric matrix with one row per support point.
`subject.index`	Integer row indices of subject visits in `X`. Repeated indices are allowed.
`method`	Density method identifier.
`graph`	Optional precomputed graph object.
`graph.control`	List of graph-method controls.
`od.control`	OD-facing alias for `density.control`.

return.details	Logical; if TRUE, keep diagnostic details in the result.
od.cv	OD-level selection mode. "none" preserves the direct fit. "visit" holds out subject visits, fits candidates on the remaining visits, and selects the candidate minimizing held-out negative log occupation mass.
visit.foldid	Optional positive integer vector assigning subject visits to OD-level cross-validation folds. Its length must equal length(subject.index).
visit.cv.folds	Number of visit folds when visit.foldid is not supplied.
visit.cv.seed	Random seed for generated visit folds.
visit.cv.epsilon	Positive floor used in held-out -log(rho[visit]) scoring.
...	Additional method-specific arguments.

Details

The "lps_logistic_binary" method name is historical. In the current OD workflow it calls fit.lps(..., outcome.family = "bernoulli"), which fits a clipped probability field with the LPS least-squares core and then converts that field to a density with normalize.density. It is not the outcome.family = "binomial" local-logistic IRLS path.

When od.cv = "visit", graph random-walk candidates may pass OD-level grids inside graph.control: walk.step.grid, affinity.method.grid, affinity.scale.grid, affinity.epsilon.grid, and normalize.grid. Missing affinity.scale values mean the usual data-derived affinity scale.

When od.cv = "visit", chart-based and LPS-family methods may pass chart.dim.grid through .... For "chart_kernel", "local_likelihood_density", "local_likelihood_bernoulli", "lps_count", "lps_logistic_binary", and "ps_lps_count", this grid compares fixed integer chart dimensions with optional "auto" and "local.auto" chart-dimension policies under the same held-out-visit negative-log-occupation score. For LPS-family OD visit CV, each outer candidate is passed to the source smoother as a scalar local model configuration; this avoids nested row-level multi-candidate selection inside each held-out-visit fold.

Value

A list of class "density_fit". Its rho component is the estimated probability mass over the rows of X, and empirical.rho is the normalized visit-count mass. The subject component summarizes the number of visits, the number of distinct visited support points, the largest visit multiplicity, and the fraction of repeatedly visited support points. Other components describe the fitted method, normalization accounting, smoothing diagnostics, and warnings as documented in fit.density. With od.cv = "visit" and return.details = TRUE, the result also contains the visit-level cross-validation table, fold assignments, and held-out predicted masses.

Examples

```
X <- matrix(seq(0, 1, length.out = 6), ncol = 1)
fit.subject.od(X, subject.index = c(1L, 3L, 3L, 6L),
               method = "empirical")
```

`get.region.boundary` *Get Boundary Vertices of a Region in a Graph*

Description

Identifies the boundary vertices of a specified region in a graph, defined as vertices in the region that have at least one neighbor outside the region.

Usage

```
get.region.boundary(adj.list, region)
```

Arguments

`adj.list`	A list of integer vectors, where each vector contains the indices of vertices adjacent to the corresponding vertex. Indices must be 1-based.
`region`	An integer vector of vertex indices (1-based) defining the region for which to find boundary vertices.

Details

This function determines which vertices in a specified region are positioned at the boundary - meaning they have at least one neighbor that is not part of the region. These boundary vertices are often treated differently in graph-based algorithms, such as harmonic smoothing, where their values are typically fixed as constraints.

The boundary definition used matches the one implemented in the C++ harmonic smoothing functions, focusing on vertices that have connections to the outside of the region.

Value

An integer vector containing the indices of the boundary vertices, which is a subset of the input `region` vector. Returns an empty integer vector if no boundary vertices exist.

See Also

`perform.harmonic.smoothing`, `harmonic.smoother`

Examples

```
# Create a simple grid graph adjacency list (5x5 grid)
create_grid_adj_list <- function(n_rows, n_cols) {
  n <- n_rows * n_cols
  adj_list <- vector("list", n)
  for (i in 1:n_rows) {
    for (j in 1:n_cols) {
      v <- (i-1) * n_cols + j
      neighbors <- numeric(0)
```

```
      # Add neighbors (up, down, left, right)
      if (i > 1) neighbors <- c(neighbors, (i-2) * n_cols + j)  # up
      if (i < n_rows) neighbors <- c(neighbors, i * n_cols + j)  # down
      if (j > 1) neighbors <- c(neighbors, (i-1) * n_cols + (j-1))  # left
      if (j < n_cols) neighbors <- c(neighbors, (i-1) * n_cols + (j+1))  # right

      adj_list[[v]] <- neighbors
    }
  }
  return(adj_list)
}

# Create a 5x5 grid graph
grid_adj_list <- create_grid_adj_list(5, 5)

# Define a region (central 3x3 subgrid)
central_region <- c(7:9, 12:14, 17:19)

# Find boundary vertices of the central region
boundary <- get.region.boundary(grid_adj_list, central_region)
print(boundary)
# Expected output: c(7, 8, 9, 12, 14, 17, 18, 19)
# (all except the center vertex 13)
```

`graph.trend.filtering.operator`

Construct a Graph Trend-Filtering Operator

Description

Builds the weighted graph difference operators used by graph trend filtering. The default `operator.family = "graph.laplacian.recursive"` uses the phase-2 recursive graph operators

$$k = 0: \quad \Delta_w^{(1)} = D_w,$$

$$k = 1: \quad \Delta_w^{(2)} = L_w = D_w^\top D_w,$$

and

$$k = 2: \quad \Delta_w^{(3)} = D_w L_w.$$

The experimental `operator.family = "path.divided.difference"` builds canonical path rows and computes position-aware finite differences along graph paths using `weight.list` as metric edge lengths.

Usage

```
graph.trend.filtering.operator(
  adj.list,
  weight.list = NULL,
```

```
  order = 0L,
  weight.rule = c("conductance", "sqrt.conductance", "unit"),
  operator.family = c("graph.laplacian.recursive", "path.divided.difference"),
  path.family = c("branch.continuation", "all.simple"),
  path.weighting = c("unit", "anchor.mean"),
  return.sparse = TRUE
)
```

Arguments

`adj.list`	List of integer neighbor vectors using 1-based vertex indices. The graph must be undirected: every edge must appear in both endpoint adjacency lists.
`weight.list`	Optional list of positive edge weights parallel to `adj.list`. For `operator.family = "graph.laplacian.recursive"`, weights are graph trend-filtering weights or conductances. For `operator.family = "path.divided.difference"`, weights are metric edge lengths used to define path coordinates. If `NULL`, all values are one.
`order`	Integer trend-filtering order. Supported values are `0L`, `1L`, and `2L`.
`weight.rule`	Character scalar. `"conductance"` uses `weight.list` directly as ω_e; `"sqrt.conductance"` uses $\sqrt{w_e}$; `"unit"` ignores `weight.list`. This applies to `operator.family = "graph.laplacian.recursive"`.
`operator.family`	Character scalar selecting the penalty operator family. The default `"graph.laplacian.recursive"` preserves the existing graph trend-filtering semantics. `"path.divided.difference"` uses local pathwise finite differences and is designed to reproduce classical one-dimensional trend filtering on path graphs.
`path.family`	Character scalar used for `operator.family = "path.divided.difference"`. `"branch.continuation"` keeps paths whose internal vertices do not pass through branch points. `"all.simple"` keeps all simple paths of the required length.
`path.weighting`	Character scalar used for `operator.family = "path.divided.difference"`. `"unit"` assigns every canonical path row weight one. `"anchor.mean"` divides rows by the number of retained canonical paths sharing the same canonical start vertex.
`return.sparse`	Logical. If `TRUE`, attach **Matrix** sparse incidence, Laplacian, and penalty matrices.

Value

A list of class `"graph.trend.filtering.operator"` containing the canonical graph, edge table, trend-filtering weights, incidence, weighted Laplacian, selected penalty operator, and nullity estimate.

Examples

```
adj <- list(2L, c(1L, 3L), c(2L, 4L), 3L)
graph.trend.filtering.operator(adj, order = 1L, weight.rule = "unit")
```

`harmonic.smoother` *Perform Harmonic Smoothing with Topology Tracking*

Description

Applies harmonic smoothing to function values defined on vertices of a graph while tracking how the topological structure (local extrema and their basins) evolves during the smoothing process. This helps identify the optimal level of smoothing that reduces noise while preserving significant features.

Usage

```
harmonic.smoother(
  adj.list,
  weight.list,
  values,
  region.vertices,
  max.iterations = 100,
  tolerance = 1e-06,
  record.frequency = 1,
  stability.window = 3,
  stability.threshold = 0.05
)
```

Arguments

`adj.list`	A list of integer vectors, where each vector contains indices of vertices adjacent to the corresponding vertex. Indices must be 1-based.
`weight.list`	A list of numeric vectors containing weights of edges corresponding to adjacencies in `adj.list`.
`values`	A numeric vector of function values defined at each vertex.
`region.vertices`	An integer vector of vertex indices (1-based) defining the region to be smoothed. Boundary vertices will have fixed values.
`max.iterations`	Integer scalar, the maximum number of relaxation iterations to perform. Default is 100.
`tolerance`	Numeric scalar, the convergence threshold for value changes. Default is 1e-6.
`record.frequency`	Integer scalar, how often to record states (every N iterations). Default is 1 (record every iteration).
`stability.window`	Integer scalar, number of consecutive iterations to check for topological stability. Default is 3.
`stability.threshold`	Numeric scalar in $[0, 1]$, maximum allowed difference in topology to consider stable. Default is 0.05.

Details

This function extends standard harmonic smoothing by monitoring the evolution of local extrema during the iterative process. It identifies a "sweet spot" where the topological structure stabilizes, indicating that noise has been removed without over-flattening important features.

The algorithm:

1. Iteratively performs harmonic smoothing on interior vertices
2. Periodically identifies local extrema and their basins
3. Monitors the stability of the topological structure
4. Identifies when the topological structure stabilizes

The function returns comprehensive information about the smoothing process, including all intermediate states and the detected stability point.

Value

A list of class `"harmonic_smoother"` containing:

`harmonic_predictions`
: Numeric vector of smoothed function values

`i_harmonic_predictions`
: Matrix of function values at each recorded iteration (columns are iterations)

`i_basins`
: List of matrices representing extrema at each iteration

`stable_iteration`
: Integer indicating the iteration at which topology stabilized

`topology_differences`
: Numeric vector of differences between consecutive recorded iterations

`basin_cx_differences`
: Alias of `topology_differences`

`converged`
: Logical indicator of whether the relaxation converged

`num_region`, `num_boundary`, `num_interior`
: Vertex counts for the requested region and its boundary/interior split

See Also

`perform.harmonic.smoothing` for basic smoothing, `plot.harmonic_smoother` for visualization methods, `summary.harmonic_smoother` for summary statistics

Examples

```
adj.list <- list(2L, c(1L, 3L), c(2L, 4L), 3L)
weight.list <- list(1, c(1, 1), c(1, 1), 1)
values <- c(0, 2, -1, 1)
result <- harmonic.smoother(
  adj.list, weight.list, values, region.vertices = seq_along(values),
  max.iterations = 20, record.frequency = 2
)
smoothed.values <- result$harmonic_predictions
smoothed.values
```

`lpl.tf.operator` *Construct a Local Polynomial Lifting Trend-Filtering Operator*

Description

Builds the Local Polynomial Lifting Trend Filtering (LPL-TF) analysis operator from local polynomial prediction residuals. For each observed target point i, the operator predicts f_i from nearby values f_j using a local polynomial model and stores the residual row

$$r_i(f) = f_i - \sum_{j \in S_i} h_{ij} f_j.$$

Usage

```
lpl.tf.operator(
  X,
  adj.list = NULL,
  weight.list = NULL,
  graph = NULL,
  graph.stage = "final",
  anchor.index = NULL,
  anchor.coordinates = NULL,
  degree = 2L,
  support.type = c("adaptive.radius", "knn", "fixed.radius"),
  support.size = NULL,
  radius = NULL,
  min.support = NULL,
  support.buffer = 3L,
  kernel = c("epanechnikov", "triangular", "gaussian", "tricube"),
  coordinate.method = c("coordinates", "local.pca"),
  chart.dim = NULL,
  support.metric = c("auto", "coordinates", "graph.geodesic"),
  auto.chart.support.metric = c("coordinates", "operator", "both"),
  auto.chart.selection.metric = c("coordinates", "operator"),
  exclude.self = TRUE,
  row.normalize = c("l2", "none", "l1"),
  local.solver = c("auto", "normal.equations", "qr", "svd"),
  normal.equations.max.condition = 1e+08,
  duplicate.action = c("keep", "error"),
  drop.rank.deficient = TRUE,
  verbose = FALSE,
  ...
)
```

Arguments

`X`	Numeric coordinate matrix with one row per observation.

adj.list, weight.list
: Optional supplied undirected graph adjacency and positive edge-length lists using 1-based vertex indices.

graph
: Optional graph object returned by dgraphs::create.rknn.graph() or a list containing adj.list/weight.list or adj_list/weight_list.

graph.stage
: Graph stage to extract from graph: "final", "raw", or "pruned".

anchor.index
: Optional integer vector of observed anchor/target indices. The current implementation supports observed anchors only.

anchor.coordinates
: Reserved for later off-observation anchors; this implementation requires NULL.

degree
: Polynomial degree. The current implementation supports 0L, 1L, and 2L.

support.type
: Coordinate support rule. "knn" uses the nearest support.size candidates including the target before self exclusion. "adaptive.radius" uses the nearest min.support positive predictors after self exclusion. "fixed.radius" uses all points within radius.

support.size
: Positive integer for support.type = "knn".

radius
: Positive coordinate radius for support.type = "fixed.radius".

min.support
: Minimum number of positive-weight predictors after self exclusion. If NULL, uses choose(ncol(X) + degree, degree) + support.buffer.

support.buffer
: Nonnegative integer added to the local polynomial design size when choosing default supports.

kernel
: Kernel used to weight local predictors by distance.

coordinate.method
: Coordinate chart used for the local polynomial design. "coordinates" uses centered ambient coordinates; "local.pca" uses a deterministic local PCA chart on the selected support.

chart.dim
: Chart dimension. For "coordinates", this must be NULL or ncol(X). For "local.pca", NULL defaults to ncol(X). The special value "auto" estimates a single chart dimension from observed-coordinate local PCA spectra only, without using responses, truth values, latent coordinates, or labels.

support.metric
: Support-distance rule. "coordinates" uses Euclidean coordinate distances; "graph.geodesic" uses shortest-path distances in the supplied graph. "auto" uses graph geodesics when a graph is supplied and coordinate distances otherwise.

auto.chart.support.metric
: Support system used when chart.dim = "auto". "coordinates" uses Euclidean coordinate neighborhoods, "operator" uses the resolved operator support metric, and "both" computes both diagnostics side by side.

auto.chart.selection.metric
: Which auto chart-dimension diagnostic to use for the fitted operator when auto.chart.support.metric = "both". The default "coordinates" preserves historical behavior.

exclude.self
: Logical. LPL-TF residual rows require TRUE.

row.normalize
: Complete-row normalization rule applied after setting target coefficient +1 and predictor coefficients -h_ij.

`local.solver` Local linear algebra rule.

`normal.equations.max.condition`
Maximum condition number for `local.solver = "auto"` to use normal equations.

`duplicate.action`
Duplicate coordinate policy.

`drop.rank.deficient`
Logical. The current implementation requires `TRUE`.

`verbose` Logical. Reserved for diagnostic messages.

`...` Reserved.

Details

The operator uses observed anchors, excludes the target point from every predictor support, and drops requested-degree rank-deficient rows with explicit metadata. There is no silent degree downgrade. Graph support distances affect support selection and kernel bandwidths only; local polynomial coordinates are controlled separately by `coordinate.method`. Graph construction is supplied by **dgraphs** or by explicit `adj.list`/`weight.list` payloads. Coordinate support paths and graph-geodesic payload validation are package-local; shortest-path distances are computed through **dgraphs**.

If a_i is the complete assembled residual row, then `row.normalize = "l2"` uses $a_i/\|a_i\|_2$, and `row.normalize = "l1"` uses $a_i/\|a_i\|_1$. Normalization is applied to the whole row, not only to predictor coefficients.

Value

A list of class `"lpl_tf_operator"` containing the sparse operator matrix `A`, row metadata, supports, local design summaries, diagnostics, settings, and the matched call.

Examples

```
X <- matrix(seq(0, 1, length.out = 18), ncol = 1)
lpl.tf.operator(X, degree = 1L, support.type = "knn",
                support.size = 7L, kernel = "gaussian")
```

---

lps.backend.diagnostics

Report LPS Backend and Chart-Dimension Diagnostics

Description

Builds a compact one-row diagnostic table for a fitted local polynomial smoother. The table records the requested backend, the backend actually used, the requested chart-dimension rule, the resolved chart dimension, selected tuning parameters, and whether the fit follows the current deployable local-PCA auto-dimension contract.

Usage

```
lps.backend.diagnostics(object)
```

Arguments

object	A fitted "lps" object.

Details

The current backend policy is conservative: backend = "auto" uses the C++ backend for ambient-coordinate LPS, but uses the R reference backend for coordinate.method = "local.pca". The native local-PCA backend "cpp.local.pca" remains an explicit opt-in backend. This helper makes that policy visible in reports and downstream experiment manifests without changing the default.

For real-data local-PCA runs, the deployable chart-dimension contract is the ordinary local.chart.method = "pca" path with chart.dim = "auto" or "local.auto" and observed-covariate auto-dimension diagnostics. In P7-style experiments this is paired with auto.chart.support.metric = "both" and auto.chart.selection.metric = "operator". The experimental "second.order.svd" chart path is reported explicitly but is not certified by this deployable local-PCA contract. For LPS itself, which uses coordinate supports, the operator-support diagnostic is currently equivalent to the coordinate-support diagnostic; the fields are still recorded so the same manifest schema can be shared with LPL-TF and S-LPL-TF experiments.

Value

A one-row data.frame with backend, chart-dimension, selection, candidate-count, and policy fields.

Examples

```
X <- matrix(seq(0, 1, length.out = 16), ncol = 1)
fit <- fit.lps(X, X[, 1]^2, support.grid = 6L, degree.grid = 1L,
               kernel.grid = "gaussian", cv.folds = 2L, backend = "R")
lps.backend.diagnostics(fit)
```

---

lps.grouped.foldid *Build a Cluster-Respecting Fold Assignment*

Description

Assigns whole clusters to cross-validation folds so that no cluster is split across folds: every observation of a cluster receives the same fold id, and therefore no training set ever shares a cluster with the fold held out against it. Folds are built by a deterministic size-balanced greedy rule: clusters are taken largest first (ties by first appearance in cluster.id) and each is placed into the currently smallest fold (ties by lowest fold index). With v equal to the number of clusters this reduces to leave-cluster-out.

Usage

```
lps.grouped.foldid(cluster.id, v = 5L, shuffle.seed = NULL)
```

Arguments

cluster.id	Vector of cluster labels (factor, character, or integer-like), one per observation, no missing values.
v	Number of folds; an integer between 2 and the number of distinct clusters.
shuffle.seed	Optional integer seed for a randomized cluster order; NULL (default) keeps the deterministic order.

Details

The assignment is fully deterministic when shuffle.seed is NULL. Supplying shuffle.seed applies one seeded permutation to the cluster order before the greedy pass (the seed is consumed immediately via set.seed), giving a reproducible randomized variant; callers following the LPS evidence conventions should record the seed they pass.

Value

An integer fold-id vector of length length(cluster.id) with values in 1:v; every fold is nonempty and every cluster maps to exactly one fold.

See Also

lps.nested.cv() for nested cross-validation that can consume grouped folds at both the outer and inner level.

Examples

```
cluster <- rep(letters[1:6], each = 2)
lps.grouped.foldid(cluster, v = 3L)
```

---

lps.nested.cv *Nested Cross-Validation for LPS with Explicit, Recorded Folds*

Description

Runs outer-fold nested cross-validation around fit.lps(): for each outer fold, candidate selection is one ordinary fit.lps call on the inner-training rows only, with an explicit inner fold id and X.eval set to the held-out outer-test rows, so the held-out fold never participates in inner selection. The pooled outer-test error is the nested generalization estimate. The same call also computes the *selected-min* arm — an ordinary fit.lps on all rows using the *same* outer.foldid — so optimism comparisons are paired on one fold assignment by construction.

Usage

```
lps.nested.cv(
  X,
  y,
  outer.foldid,
  fit.args = list(),
  inner.folds = 5L,
  cluster.id = NULL,
  inner.foldid.method = c("round.robin", "grouped"),
  inner.shuffle.seed = NULL
)
```

Arguments

X	Numeric matrix of observations (rows) used for training.
y	Numeric response vector with length(y) == nrow(X).
outer.foldid	Positive integer vector of length nrow(X) assigning rows to outer folds (at least two distinct folds).
fit.args	Named list of additional arguments passed to every fit.lps call (grids, backend, design settings, ...). Must not contain X, y, foldid, or X.eval: the fold plumbing is owned by this function so both arms see the same folds.
inner.folds	Number of inner selection folds (integer >= 2).
cluster.id	Optional cluster labels (length nrow(X)), required for inner.foldid.method = "grouped".
inner.foldid.method	Inner fold construction: "round.robin" (default) or "grouped" (cluster-respecting).
inner.shuffle.seed	Optional integer; per-fold offset seed for the randomized variants described above. Recorded in the return value.

Details

The existing fit.lps behavior is untouched: this utility consumes the public API with explicit foldid only. It currently supports outcome.family = "gaussian" (the default) and scores with RMSE.

Inner folds are built per outer fold and fully recorded in the return value: "round.robin" assigns rep_len(1:inner.folds, n) over the inner-training rows in row order (deterministic; if inner.shuffle.seed is supplied, fold k — by position — uses set.seed(inner.shuffle.seed + k) and permutes the balanced assignment, giving a reproducible randomized variant); "grouped" builds cluster-respecting inner folds with lps.grouped.foldid() on the inner-training rows of cluster.id (passing the same per-fold offset seed when inner.shuffle.seed is supplied).

Value

A list of class "lps_nested_cv":

nested.rmse pooled RMSE of the outer-test predictions over all rows with finite predictions.

`n.missing.predictions` count of non-finite outer-test predictions (e.g. `unstable.action = "na"` fallbacks).

`folds` one row per outer fold: fold label, test size, selected `support.size` / `degree` / `kernel` / `bandwidth.multiplier`, the inner selected-min CV score, and the fold's outer-test RMSE.

`predictions` length-`nrow(X)` vector of outer-test predictions (each row predicted by the fold that held it out).

`selected.min` the paired selected-min arm on the same `outer.foldid`: `selected` (the `fit.lps` selected row), `cv.score` (its observed CV RMSE), `foldid`, and `fit` (the full-data `fit.lps` object, usable for deployment on an external test set).

`outer.foldid`, `test.index`, `train.index`, `inner.foldid`, `inner.foldid.used`, `inner.cv.table` complete fold/index telemetry: the realized inner fold ids as constructed and as recorded by each inner `fit.lps` (`$foldid`), per-fold index sets, and each fold's full inner CV candidate table.

`outer.cluster.whole` `TRUE`/`FALSE` whether every cluster lies wholly inside one outer fold (`NA` when `cluster.id` is absent).

`inner.folds`, `inner.foldid.method`, `inner.shuffle.seed`, `fit.args`, `call` the recorded configuration.

See Also

`lps.grouped.foldid()` for the grouped fold constructor.

Examples

```
X <- matrix(seq(0, 1, length.out = 18), ncol = 1)
y <- sin(2 * pi * X[, 1])
nested <- lps.nested.cv(
  X, y, outer.foldid = rep(1:3, length.out = 18), inner.folds = 2L,
  fit.args = list(support.grid = 6L, degree.grid = 1L,
                  kernel.grid = "gaussian", backend = "R")
)
nested$rmse
```

---

lps.pointwise.band *Pointwise Variance and Confidence Band for a Fixed-Configuration LPS Fit*

Description

Computes, from the analytically extracted linear-smoother matrix `S` of a fixed-configuration LPS fit (see `lps.smoother.matrix()`), the pointwise variance `Var(fitted_i) = sigma^2 * sum_j S_ij^2`, the effective degrees of freedom `df = tr(S)`, the plug-in noise estimate `sigma.hat^2 = RSS / (n - tr(S))`, and the pointwise confidence band `fitted_i +/- z * sigma * ||S_i.||_2` with `z = qnorm(1 - (1 - level) / 2)`.

Usage

```
lps.pointwise.band(object, sigma = NULL, level = 0.95, check.tol = 1e-10)
```

Arguments

object	A fitted "lps" object from fit.lps() at a fixed configuration, with X.eval identical to X.
sigma	Known noise standard deviation (positive scalar), or NULL (default) to use the plug-in sigma.hat.
level	Confidence level of the band, a single number strictly between 0 and 1. Default 0.95.
check.tol	Passed to lps.smoother.matrix()'s self-guard.

Details

With sigma supplied (known noise standard deviation), the band uses it directly (sigma.source = "known"); with sigma = NULL the plug-in sigma.hat is used (sigma.source = "plug.in"). sigma.hat is reported in both modes. The variance is purely the linear-smoother sampling variance: the band makes no bias correction, so where bias dominates (boundary, high curvature) undercoverage is expected and must be reported, not masked.

Requires X.eval identical to X (the square training-fit smoother, on which tr(S) and RSS are defined), in addition to all restrictions of lps.smoother.matrix(). If any evaluation point's local fit returned NA, its variance/band entries are NA, and df, rss, and sigma.hat are NA as well; supplying a known sigma still yields bands at the unaffected points.

Value

A list of class "lps.pointwise.band" with named fields: fitted (the fit's raw fitted values), se, variance, lower, upper, level, z, sigma (the supplied known sigma, or NA in plug-in mode), sigma.hat, sigma.source ("known" or "plug.in"), df (tr(S)), rss, n.train, smoother.row.norm (||S_i.||_2), and configuration (the pinned fit configuration).

See Also

lps.smoother.matrix()

Examples

```
set.seed(1)
n <- 30
X <- matrix(runif(2 * n, -1, 1), ncol = 2)
y <- sin(pi * X[, 1]) + 0.1 * rnorm(n)
fit <- fit.lps(X, y, foldid = rep(1:2, length.out = n),
               support.grid = 12L, degree.grid = 1L,
               kernel.grid = "tricube", backend = "R",
               design.basis = "orthogonal.polynomial.drop",
               ridge.multiplier.grid = 0, ridge.condition.max = Inf,
               unstable.action = "na")
band.known <- lps.pointwise.band(fit, sigma = 0.1)
```

```
band.plugin <- lps.pointwise.band(fit)
band.known$df
band.plugin$sigma.hat
```

`lps.smoother.matrix` *Extract the Linear-Smoother Matrix of a Fixed-Configuration LPS Fit*

Description

For a fixed configuration (singleton `support.grid`, `degree.grid`, and `kernel.grid`, with an explicit numeric chart dimension) the LPS fitted vector is linear in the response: `fitted = S %*% y` with `S` depending on `X`, the kernel weights, and the configuration, but not on `y`. This function reconstructs `S` analytically, one evaluation row at a time, by rebuilding each local fit's support, kernel weights, local chart, and design through the same internal routines `fit.lps()` used, and reading off the influence row of the local weighted least-squares solve.

Usage

```
lps.smoother.matrix(object, check.tol = 1e-10)
```

Arguments

`object`	A fitted `"lps"` object from `fit.lps()` at a fixed configuration (see Details).
`check.tol`	Positive scalar: maximum allowed absolute discrepancy of the self-guard identity `S %*% y == fitted.values.raw`. Default `1e-10`, the program's algebraic tolerance.

Details

The extraction refuses configurations where the linearity premise fails or is unsupported: it requires `outcome.family = "gaussian"`, the R backend, `design.basis = "orthogonal.polynomial.drop"`, singleton grids (no data-driven selection: the CV-selected pipeline is *not* a linear smoother), and `coordinate.method = "coordinates"` or `"local.pca"` with an explicit numeric `chart.dim` (never `"auto"` or `"local.auto"`).

Self-guard: before returning, the function verifies `max(abs(S %*% y - fitted.values.raw)) <= check.tol` against the fit it was given (and that the `NA` patterns agree), so any divergence between the reconstruction and the estimator is a hard error, never a silent drift.

Local fits that fell back are represented honestly: a weighted-mean fallback (`unstable.action = "mean"`) contributes its exact linear row `w / sum(w)`; an `unstable.action = "na"` non-fit contributes an all-`NA` row.

Value

A numeric matrix `S` with `nrow(object$X.eval)` rows and `nrow(object$X)` columns: row `i` holds the weights through which the training responses enter the prediction at evaluation point `i`.

See Also

lps.pointwise.band() for pointwise variances and confidence bands derived from S.

Examples

```
set.seed(1)
n <- 30
X <- matrix(runif(2 * n, -1, 1), ncol = 2)
y <- sin(pi * X[, 1]) + 0.1 * rnorm(n)
fit <- fit.lps(X, y, foldid = rep(1:2, length.out = n),
               support.grid = 12L, degree.grid = 1L,
               kernel.grid = "tricube", backend = "R",
               design.basis = "orthogonal.polynomial.drop",
               ridge.multiplier.grid = 0, ridge.condition.max = Inf,
               unstable.action = "na")
S <- lps.smoother.matrix(fit)
max(abs(S %*% y - fit$fitted.values))   # ~1e-15: the linear identity
sum(diag(S))                            # effective degrees of freedom
```

---

malps.gcv *Compute MALPS Linear-Smoother Diagnostics*

Description

Computes effective degrees of freedom, generalized cross-validation (GCV), and analytic leave-one-out residual diagnostics from a MALPS smoother matrix. These diagnostics are exact for fixed-support, fixed-weight linear MALPS fits. For cross-validated fits they are conditional on the selected support profile. Robust fits are rejected by default for the same reason described in malps.smoother.matrix.

Usage

```
malps.gcv(
  object,
  y = NULL,
  smoother.matrix = NULL,
  include.loocv = TRUE,
  max.n = 1000L,
  allow.robust = FALSE,
  ...
)
```

Arguments

object	A "malps" object from fit.malps or refit.malps.
y	Optional response vector. Defaults to object$y.
smoother.matrix	Optional precomputed matrix from malps.smoother.matrix.

include.loocv	Logical; include analytic leave-one-out residuals and mean squared error.
max.n	Maximum dense smoother size passed to malps.smoother.matrix when smoother.matrix = NULL.
allow.robust	Logical; passed to malps.smoother.matrix.
...	Reserved for future extensions.

Details

The GCV score is computed as

$$\mathrm{GCV} = \frac{n^{-1}\|y - Sy\|_2^2}{(1 - \mathrm{tr}(S)/n)^2}.$$

The analytic leave-one-out residuals are computed as

$$e_i^{\mathrm{loo}} = \frac{y_i - \hat{y}_i}{1 - S_{ii}}.$$

Value

A list with residual, fitted-value, EDF, GCV, and optional LOOCV diagnostics.

Examples

```
X <- matrix(seq(0, 1, length.out = 20), ncol = 1)
fit <- fit.malps(X, X[, 1]^2, degree = 1L,
                 support.type = "knn", support.size = 8L)
malps.gcv(fit)$gcv
```

---

malps.smoother.matrix *Construct The Conditional MALPS Smoother Matrix*

Description

Constructs the exact training-point smoother matrix for a fitted fit.malps object, conditional on the stored supports, local charts, fitting weights, and averaging weights. For a non-robust MALPS fit or weighted refit with fixed supports, the returned matrix S satisfies $\hat{y} = Sy$. If the original fit used cross-validation, this matrix is conditional on the selected support profile; it does not account for the response-dependence of the model-selection step.

Usage

```
malps.smoother.matrix(object, max.n = 1000L, allow.robust = FALSE, ...)
```

Arguments

`object`	A `"malps"` object from `fit.malps` or `refit.malps`.
`max.n`	Maximum number of training observations for which a dense smoother matrix may be constructed. Use `Inf` to disable this guard.
`allow.robust`	Logical; allow fixed-final-weight linearization for fits with `robust.iterations > 0L`.
`...`	Reserved for future extensions.

Details

Robust residual reweighting makes the effective fitting weights depend on the response. By default this function therefore rejects robust MALPS fits. Setting `allow.robust = TRUE` constructs the fixed-final-weight linearization, which reproduces the stored fit but should not be interpreted as the exact response-to-fit map.

Value

A dense numeric $n \times n$ matrix with attributes describing whether the matrix is conditional on support selection and whether it used a robust fixed-weight linearization.

Examples

```
X <- matrix(seq(0, 1, length.out = 20), ncol = 1)
fit <- fit.malps(X, X[, 1]^2, degree = 1L,
                 support.type = "knn", support.size = 8L)
S <- malps.smoother.matrix(fit)
max(abs(S %*% fit$y - fit$fitted.values))
```

`materialize.synthetic` *Materialize a synthetic-data specification*

Description

Materialize a synthetic-data specification

Usage

```
materialize.synthetic(
  spec,
  n = NULL,
  seed,
  rng.policy = c("named.stream.v1", "legacy"),
  validate = TRUE
)
```

Arguments

spec	A synthetic_spec.
n	Sample size, or NULL for fixed-size sampling.
seed	Scalar whole-number seed.
rng.policy	Versioned RNG policy.
validate	Whether to validate the returned dataset.

Value

A synthetic_dataset.

Examples

```
spec <- synthetic.registry.spec("G1")
materialize.synthetic(spec, n = 20L, seed = 1L)
```

---

materialize.synthetic.instance

Materialize a frozen synthetic instance

Description

Materialize a frozen synthetic instance

Usage

```
materialize.synthetic.instance(instance.id, validate = TRUE)
```

Arguments

instance.id	Frozen instance ID.
validate	Whether to validate and checksum the result.

Value

A synthetic_dataset whose dataset.id is instance.id.

Examples

```
materialize.synthetic.instance("geosmooth.g1.default.v1")
```

`metric.graph.heat.eta.grid` *Construct a Graph Heat-Time Grid*

Description

Creates a positive heat-time grid from a `"metric.graph.lowpass.basis"` object.

Usage

```
metric.graph.heat.eta.grid(
  basis,
  rule = c("spectral_guarded", "w1_inverse_spectrum"),
  n.initial = 40L,
  include.zero = FALSE,
  truncation.tol = 1e-04,
  equilibrium.tol = 1e-04
)
```

Arguments

`basis`	A `"metric.graph.lowpass.basis"` object.
`rule`	Grid rule. `"w1_inverse_spectrum"` requires a complete basis and reproduces the W1 inverse-spectrum grid. `"spectral_guarded"` raises the lower endpoint for a truncated basis until the conservative omitted-mode attenuation bound is no larger than `truncation.tol`, and extends the upper endpoint until the slowest retained positive mode is attenuated to `equilibrium.tol`.
`n.initial`	Number of positive grid values.
`include.zero`	Logical. Include the exact no-smoothing endpoint.
`truncation.tol`	Positive tolerance smaller than one for the conservative omitted-mode attenuation bound.
`equilibrium.tol`	Positive tolerance smaller than one for the slowest positive retained mode at the upper endpoint.

Value

A numeric vector with grid-construction metadata stored as attributes.

Examples

```
adj <- list(2L, c(1L, 3L), c(2L, 4L), 3L)
lengths <- list(1, c(1, 1), c(1, 1), 1)
basis <- metric.graph.lowpass.basis(adj, lengths, n.eigenpairs = 4L,
                                    eigen.solver = "dense")
metric.graph.heat.eta.grid(basis, n.initial = 6L)
```

`metric.graph.heat.extend.lower` *Propose a Guarded Lower Graph Heat Time*

Description

Proposes one lower positive heat time after an external search controller has classified the current lower endpoint. The helper enforces a geometric expansion step, an identity-departure floor, a maximum number of expansion rounds, and the truncated-basis resolution certificate. It does not decide whether an endpoint is competitive; fold-level or cohort-level search logic remains the caller's responsibility.

Usage

```
metric.graph.heat.extend.lower(
  basis,
  eta.grid,
  endpoint.status = c("active", "inactive", "unresolved"),
  expansion.factor = 3,
  max.expansions = 3L,
  expansions.completed = 0L,
  identity.departure = 0.01,
  truncation.tol = 1e-04,
  unresolved.action = c("error", "mark")
)
```

Arguments

`basis`	A `"metric.graph.lowpass.basis"` object.
`eta.grid`	Current finite positive heat-time grid. The exact identity time `eta = 0` is intentionally excluded from competitive search.
`endpoint.status`	External lower-endpoint classification: `"active"` proposes one extension, while `"inactive"` and `"unresolved"` return the grid unchanged.
`expansion.factor`	Finite numeric factor greater than one. An active proposal is `min(eta.grid) / expansion.factor` before applying the identity floor.
`max.expansions`	Nonnegative integer maximum number of lower-extension rounds.
`expansions.completed`	Nonnegative integer number of extension rounds already admitted under the same search contract.
`identity.departure`	Positive number smaller than one. The proposed time cannot be smaller than `-log(1 - identity.departure) / lambda.max`, where `lambda.max` is the largest retained eigenvalue. For a complete basis this is the exact largest graph-Laplacian eigenvalue.

`truncation.tol` Positive tolerance smaller than one for the conservative omitted-mode attenuation bound.

`unresolved.action` Action when an active proposal is not certified by a truncated basis: `"error"` or `"mark"`.

Value

A list of class `"metric.graph.heat.lower.extension"` with the augmented or unchanged grid and proposal telemetry. A proposal is added only when `admitted` is `TRUE`.

Examples

```
adj <- list(2L, c(1L, 3L), c(2L, 4L), 3L)
lengths <- list(1, c(1, 1), c(1, 1), 1)
basis <- metric.graph.lowpass.basis(adj, lengths, n.eigenpairs = 4L,
                                    eigen.solver = "dense")
eta <- metric.graph.heat.eta.grid(basis, n.initial = 6L)
metric.graph.heat.extend.lower(basis, eta, endpoint.status = "active")
```

---

metric.graph.lowpass.basis

Construct a Reusable Metric Graph Low-Pass Spectral Basis

Description

Builds a metric-conductance graph Laplacian and computes the low-frequency eigensystem used by graph low-pass filters. The resulting object is response-independent and can be reused for many responses and filter parameters.

Usage

```
metric.graph.lowpass.basis(
  adj.list,
  weight.list,
 conductance.rule = c("inverse.length.power", "exp.length", "exp.length.squared",
    "self.tuned.gaussian"),
  conductance.epsilon = 1e-08,
  conductance.alpha = 1,
  conductance.sigma = NULL,
  conductance.sigma.rule = c("edge.quantile", "median", "local.k"),
  conductance.sigma.quantile = 0.75,
  conductance.local.k = 5L,
  laplacian.type = c("unnormalized", "symmetric.normalized"),
  n.eigenpairs = 50L,
  eigen.solver = c("auto", "sparse", "dense"),
  dense.eigen.threshold = 200L,
  dense.fallback.threshold = 5000L,
```

```
  dense.fallback = c("auto", "never", "always"),
  verbose = FALSE
)
```

Arguments

`adj.list`	List of integer neighbor vectors using 1-based vertex indices.
`weight.list`	List of positive metric edge lengths parallel to `adj.list`. These are interpreted as edge lengths, not conductances.
`conductance.rule`	Character scalar. One of `"inverse.length.power"`, `"exp.length"`, `"exp.length.squared"`, or `"self.tuned.gaussian"`.
`conductance.epsilon`	Positive numeric regularizer used by inverse-power conductances and as a local-scale floor.
`conductance.alpha`	Positive numeric exponent for `"inverse.length.power"`.
`conductance.sigma`	Optional positive global scale for exponential rules. If `NULL`, it is selected by `conductance.sigma.rule`.
`conductance.sigma.rule`	Rule for selecting a global scale when needed.
`conductance.sigma.quantile`	Quantile used when `conductance.sigma.rule = "edge.quantile"`.
`conductance.local.k`	Positive integer local incident-edge order statistic for `"self.tuned.gaussian"`.
`laplacian.type`	Laplacian operator. `"unnormalized"` uses the weighted graph Laplacian $L = D - C$. `"symmetric.normalized"` uses $L_{\mathrm{sym}} = I - D^{-1/2} C D^{-1/2}$.
`n.eigenpairs`	Positive integer number of eigenpairs to compute.
`eigen.solver`	`"auto"`, `"sparse"`, or `"dense"`.
`dense.eigen.threshold`	Exact dense threshold for auto mode.
`dense.fallback.threshold`	Maximum graph size for emergency dense fallback when sparse decomposition fails and fallback is allowed.
`dense.fallback`	`"auto"`, `"never"`, or `"always"`.
`verbose`	Logical. Reserved for future diagnostic messages.

Details

The basis is complete only when it contains one eigenvector per graph vertex. A truncated basis represents only the retained low-frequency subspace. The largest retained eigenvalue supplies a conservative proxy for bounding the contribution of omitted modes because all omitted eigenvalues are at least as large.

Value

A list of class "metric.graph.lowpass.basis" containing the graph operator, eigenvalues, eigenvectors, solver metadata, and spectral completeness diagnostics.

Examples

```
adj <- list(2L, c(1L, 3L), c(2L, 4L), 3L)
lengths <- list(1, c(1, 1), c(1, 1), 1)
metric.graph.lowpass.basis(adj, lengths, n.eigenpairs = 4L,
                           eigen.solver = "dense")
```

---

metric.graph.lowpass.operator

Construct a Metric-Conductance Graph Low-Pass Operator

Description

Builds a weighted graph Laplacian by transforming metric edge lengths into conductances. This operator is a direct metric-conductance comparator to the legacy rdgraph regression smoother, not a replacement for the Riemannian-complex/overlap-density smoother.

Usage

```
metric.graph.lowpass.operator(
  adj.list,
  weight.list,
 conductance.rule = c("inverse.length.power", "exp.length", "exp.length.squared",
    "self.tuned.gaussian"),
  conductance.epsilon = 1e-08,
  conductance.alpha = 1,
  conductance.sigma = NULL,
  conductance.sigma.rule = c("edge.quantile", "median", "local.k"),
  conductance.sigma.quantile = 0.75,
  conductance.local.k = 5L,
  laplacian.type = c("unnormalized", "symmetric.normalized"),
  return.sparse = TRUE,
  verbose = FALSE
)
```

Arguments

adj.list	List of integer neighbor vectors using 1-based vertex indices.
weight.list	List of positive metric edge lengths parallel to adj.list. These are interpreted as edge lengths, not conductances.
conductance.rule	Character scalar. One of "inverse.length.power", "exp.length", "exp.length.squared", or "self.tuned.gaussian".

`conductance.epsilon`
: Positive numeric regularizer used by inverse-power conductances and as a local-scale floor.

`conductance.alpha`
: Positive numeric exponent for `"inverse.length.power"`.

`conductance.sigma`
: Optional positive global scale for exponential rules. If `NULL`, it is selected by `conductance.sigma.rule`.

`conductance.sigma.rule`
: Rule for selecting a global scale when needed.

`conductance.sigma.quantile`
: Quantile used when `conductance.sigma.rule = "edge.quantile"`.

`conductance.local.k`
: Positive integer local incident-edge order statistic for `"self.tuned.gaussian"`.

`laplacian.type`
: Laplacian operator. `"unnormalized"` uses the weighted graph Laplacian $L = D - C$. `"symmetric.normalized"` uses $L_{\mathrm{sym}} = I - D^{-1/2} C D^{-1/2}$.

`return.sparse`
: Logical. If `TRUE`, attach a **Matrix** sparse Laplacian when **Matrix** is available.

`verbose`
: Logical. Reserved for future diagnostic messages.

Details

The legacy rdgraph regression precomputed-graph path uses supplied `weight.list` values as edge lengths for neighborhood ordering. The spectral conductance in that smoother is overlap-density based:

$$c_e^{\rho} = 1/\max(\rho_1(e), 10^{-10}),$$

where $\rho_1(e)$ is computed by the Riemannian-complex density machinery.

This function instead constructs conductances directly from metric lengths:

$$c_{ij} = \phi(\ell_{ij}).$$

Supported phase-1 transforms are

$$c_{ij} = (\ell_{ij} + \epsilon)^{-\alpha},$$

$$c_{ij} = \exp(-\ell_{ij}/\sigma),$$

$$c_{ij} = \exp(-\ell_{ij}^2/\sigma^2),$$

and

$$c_{ij} = \exp(-\ell_{ij}^2/(\sigma_i \sigma_j)).$$

For `laplacian.type = "symmetric.normalized"`, smoothing is performed in the Euclidean eigenbasis of L_{sym}. The null vector is proportional to $\sqrt{d}$, not the constant vector, so this mode does not preserve constant responses in the same way as the unnormalized Laplacian.

Value

A list of class `"metric.graph.lowpass.operator"` containing the edge table, conductances, degree vector, Laplacian triplets, summaries, and optionally a sparse Laplacian matrix.

Examples

```
adj <- list(2L, c(1L, 3L), c(2L, 4L), 3L)
lengths <- list(1, c(1, 1), c(1, 1), 1)
metric.graph.lowpass.operator(adj, lengths)
```

`normalize.density` *Normalize Fitted Values Into a Density*

Description

Converts a numeric field or fitted smoother/regression object into a probability mass vector over the evaluation support. This is the explicit adapter between ordinary smoothers such as `fit.lps`, `fit.ps.lps`, and `fit.metric.graph.lowpass` and density or occupation-density workflows.

Usage

```
normalize.density(x, ...)

## S3 method for class 'numeric'
normalize.density(
  x,
  X = NULL,
  density.control = list(),
  method.id = "normalized_numeric",
  keep.source.fit = FALSE,
  adj.list = NULL,
  empirical.rho = NULL,
  return.details = TRUE,
  ...
)

## Default S3 method:
normalize.density(
  x,
  X = NULL,
  density.control = list(),
  method.id = NULL,
  keep.source.fit = TRUE,
  adj.list = NULL,
  empirical.rho = NULL,
  return.details = TRUE,
  ...
)

## S3 method for class 'lps'
normalize.density(
  x,
```

```
  X = NULL,
  density.control = list(),
  method.id = NULL,
  keep.source.fit = TRUE,
  adj.list = NULL,
  empirical.rho = NULL,
  return.details = TRUE,
  ...
)

## S3 method for class 'ps_lps'
normalize.density(
  x,
  X = NULL,
  density.control = list(),
  method.id = NULL,
  keep.source.fit = TRUE,
  adj.list = NULL,
  empirical.rho = NULL,
  return.details = TRUE,
  ...
)

## S3 method for class 'metric.graph.lowpass.fit'
normalize.density(
  x,
  X = NULL,
  density.control = list(),
  method.id = NULL,
  keep.source.fit = TRUE,
  adj.list = NULL,
  empirical.rho = NULL,
  return.details = TRUE,
  ...
)

## S3 method for class 'metric.graph.lowpass.refit'
normalize.density(
  x,
  X = NULL,
  density.control = list(),
  method.id = NULL,
  keep.source.fit = TRUE,
  adj.list = NULL,
  empirical.rho = NULL,
  return.details = TRUE,
  ...
)
```

Arguments

x	Numeric vector or fitted object with a fitted.values field.
...	Additional arguments passed to methods.
X	Optional support/evaluation matrix. If omitted, methods use the fitted object's stored X.eval or X field when available; for a bare numeric vector, a one-dimensional index support is used.
density.control	List controlling clipping, normalization, and accounting checks. See fit.density.
method.id	Character method identifier recorded in the returned object.
keep.source.fit	Logical; if TRUE, retain the source fit in diagnostics for object methods.
adj.list	Optional adjacency list used to compute graph-local smoothness diagnostics for the normalized density.
empirical.rho	Optional empirical probability mass vector used for accounting diagnostics.
return.details	Logical; if TRUE, keep diagnostic details in the result.

Value

A list of class "density_fit".

Examples

```
normalize.density(c(0.5, -0.1, 0.6, 0), X = matrix(1:4, ncol = 1))
```

---

perform.harmonic.smoothing

Perform Harmonic Smoothing on Graph Function Values

Description

Applies harmonic smoothing to function values defined on vertices of a graph, preserving values at the boundary of a specified region while smoothly interpolating interior values. This function implements a discrete Laplace equation solution using weighted averaging.

Usage

```
perform.harmonic.smoothing(
  adj.list,
  weight.list,
  values,
  region.vertices,
  max.iterations = 100,
  tolerance = 1e-06
)
```

Arguments

`adj.list`	A list of integer vectors, where each vector contains indices of vertices adjacent to the corresponding vertex. Indices must be 1-based.
`weight.list`	A list of numeric vectors containing weights of edges corresponding to adjacencies in `adj.list`.
`values`	A numeric vector of function values defined at each vertex.
`region.vertices`	An integer vector of vertex indices (1-based) defining the region to be smoothed. Boundary vertices will have fixed values.
`max.iterations`	Integer scalar, the maximum number of relaxation iterations to perform. Default is 100.
`tolerance`	Numeric scalar, the convergence threshold for value changes. Default is 1e-6.

Details

Harmonic smoothing preserves the overall shape of a function defined on a graph while removing local fluctuations. It works by iteratively updating interior vertex values as weighted averages of their neighbors until convergence, while keeping boundary values fixed.

The algorithm:

1. Identifies boundary vertices (vertices with neighbors outside the region or degree 1 vertices)
2. Iteratively updates interior vertex values using edge-weighted averaging
3. Continues until convergence or maximum iterations reached

Edge weights are incorporated by using their inverse as weighting factors, respecting the geometric structure of the graph.

Value

A list containing:

- `harmonic_predictions`: the numeric vector of smoothed values;
- `converged`: whether both the maximum update and discrete harmonic residual fell below `tolerance`;
- `num_region`, `num_boundary`, and `num_interior`: vertex counts for the requested region and its boundary/interior split;
- `num_iterations`: the number of relaxation iterations run;
- `max_change` and `max_residual`: per-iteration convergence diagnostics.

See Also

`harmonic.smoother` for smoothing with topology tracking, `get.region.boundary` for boundary vertex identification

Examples

```
adj.list <- list(2L, c(1L, 3L), c(2L, 4L), 3L)
weight.list <- list(1, c(1, 1), c(1, 1), 1)
values <- c(0, 2, -1, 1)
result <- perform.harmonic.smoothing(
  adj.list, weight.list, values, region.vertices = 1:3
)
result$harmonic_predictions
```

`plot.harmonic_smoother` *Plot Method for Harmonic Smoother Results*

Description

Creates various plots to visualize the results of harmonic smoothing with topology tracking.

Usage

```
## S3 method for class 'harmonic_smoother'
plot(x, y = NULL, ..., type = c("topology", "extrema", "values"))
```

Arguments

`x`	An object of class `"harmonic_smoother"`.
`y`	Ignored (included for S3 method consistency).
`...`	Additional graphical parameters passed to `plot()`.
`type`	Character string specifying the type of plot. Options are: **"topology"** Evolution of topology differences (default) **"extrema"** Evolution of extrema counts **"values"** Original vs smoothed values

Value

Invisibly returns the input object.

See Also

`harmonic.smoother`

Examples

```
adj.list <- list(2L, c(1L, 3L), c(2L, 4L), 3L)
weight.list <- list(1, c(1, 1), c(1, 1), 1)
values <- c(0, 2, -1, 1)
result <- harmonic.smoother(
  adj.list, weight.list, values, region.vertices = seq_along(values),
  max.iterations = 20, record.frequency = 2
)
plot(result, type = "values")
```

`plot.synthetic_dataset` *Plot a canonical synthetic dataset*

Description

One-dimensional datasets show response and truth against the first latent coordinate. Higher-dimensional datasets show the first two predictor coordinates, colored by response or region.

Usage

```
## S3 method for class 'synthetic_dataset'
plot(x, color = c("response", "truth", "region"), ...)
```

Arguments

`x`	A `synthetic_dataset`.
`color`	Color mapping: response, truth, or region.
`...`	Additional arguments passed to `graphics::plot()`.

Value

`x`, invisibly.

`predict.lpl_tf` *Predict From A Local Polynomial Lifting Trend Filter*

Description

Predict From A Local Polynomial Lifting Trend Filter

Usage

```
## S3 method for class 'lpl_tf'
predict(
  object,
  newdata = NULL,
  type = c("response"),
  allow.incomplete = FALSE,
  ...
)
```

Arguments

object	A "lpl_tf" object.
newdata	Must be NULL in Phase 2.
type	Prediction type. Phase 2 supports only "response".
allow.incomplete	Reserved.
...	Reserved.

Value

Fitted values at the training points.

---

predict.lps *Predict from an LPS Fit*

Description

Predict from an LPS Fit

Usage

```
## S3 method for class 'lps'
predict(object, newdata = NULL, type = c("response", "raw"), ...)
```

Arguments

object	A fitted "lps" object.
newdata	Optional prediction matrix. Defaults to the fitted object's stored X.eval.
type	Prediction scale. "response" returns response-scale predictions; for outcome.family = "bernoulli" or "binomial" these are probabilities in [0,1]. "raw" returns the unmodified local least-squares predictions for "bernoulli" and the fitted probabilities for "binomial".
...	Unused.

Value

A numeric vector of predictions.

`predict.malps` *Predict From A MALPS Fit*

Description

Predict From A MALPS Fit

Usage

```
## S3 method for class 'malps'
predict(
  object,
  newdata = NULL,
  type = c("response"),
  allow.incomplete = FALSE,
  ...
)
```

Arguments

`object`	A `"malps"` object from `fit.malps`.
`newdata`	Optional numeric coordinate matrix with the same number of columns as `object$X`. If `NULL`, returns stored training-point fitted values. New-point prediction is currently implemented for coordinate-support fits only; it fails informatively for objects fitted with `support.metric = "graph.geodesic"` because new targets need a graph-attachment/geodesic-distance contract.
`type`	Prediction type. Currently only `"response"`.
`allow.incomplete`	Logical; if `FALSE`, new-point prediction fails when any target has no positive averaging coverage. If `TRUE`, those targets receive `NA_real_`.
`...`	Reserved for future extensions.

Value

Numeric vector of fitted values.

predict.slpl_tf *Predict From A Fixed-Operator Synchronized LPL-TF Model*

Description

Predict From A Fixed-Operator Synchronized LPL-TF Model

Usage

```
## S3 method for class 'slpl_tf'
predict(object, newdata = NULL, type = c("response"), ...)
```

Arguments

object	A "slpl_tf" fit.
newdata	Must be NULL in Phase S2.
type	Prediction type. Phase S2 supports only "response".
...	Reserved.

Value

Fitted values at the training points.

print.harmonic_smoother *Print Method for Harmonic Smoother Results*

Description

Prints a concise summary of harmonic smoother results.

Usage

```
## S3 method for class 'harmonic_smoother'
print(x, ...)
```

Arguments

x	An object of class "harmonic_smoother".
...	Further arguments passed to or from other methods.

Value

Invisibly returns the input object.

See Also

harmonic.smoother, summary.harmonic_smoother

---

print.summary.harmonic_smoother

Print Method for Summary of Harmonic Smoother Results

Description

Prints the summary of harmonic smoother results in a formatted manner.

Usage

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

Arguments

x	An object of class "summary.harmonic_smoother".
...	Further arguments passed to or from other methods.

Value

Invisibly returns the input object.

See Also

summary.harmonic_smoother

---

print.synthetic_dataset

Print a canonical synthetic dataset

Description

Print a canonical synthetic dataset

Usage

```
## S3 method for class 'synthetic_dataset'
print(x, ...)
```

Arguments

x	A synthetic_dataset.
...	Ignored.

Value

x, invisibly.

`pttf.geometry` *Construct PTTF Local Geometry*

Description

Builds the geometry layer for the experimental parallel-transport trend filtering (PTTF) route. The returned object contains graph supports, local PCA tangent frames, edge directions, orthogonal edge transports, sampling density metadata, and diagnostics. It does not assemble transported difference operators and it does not fit a response.

Usage

```
pttf.geometry(
  X,
  adj.list = NULL,
  weight.list = NULL,
  graph = c("rknn", "supplied"),
  tangent.dim,
  local.support = c("graph.disk", "neighbors"),
  min.support = NULL,
  max.hops = 3L,
  support.k = NULL,
  graph.k.scale = 1L,
  graph.radius.factor = 1,
  graph.radius.rule = "geomean",
  transport.rule = c("procrustes"),
  synchronize.orientation = TRUE,
  density.method = c("support.radius"),
  alpha = 1,
  diagnostics = TRUE
)
```

Arguments

`X`	Numeric data matrix with one row per vertex.
`adj.list`	Optional supplied graph adjacency list using 1-based vertex indices.
`weight.list`	Optional positive edge-length list parallel to `adj.list`.
`graph`	Graph source. `"rknn"` builds an adaptive-radius graph from `X`; `"supplied"` uses `adj.list` and `weight.list`.
`tangent.dim`	Fixed global tangent dimension for phase-1 geometry.
`local.support`	Local support construction rule. `"graph.disk"` uses graph-hop disks; `"neighbors"` starts from the closed one-hop neighborhood and tops up by graph-hop expansion.

`min.support` Minimum support size. Defaults to $\max(2m+2, m+3)$, where $m =$ `tangent.dim`.

`max.hops` Maximum hop radius used when topping up local supports.

`support.k` Optional cap on local support size after top-up. The center vertex is always retained and remaining vertices are selected by graph metric distance, with vertex-index tie breaking.

`graph.k.scale`, `graph.radius.factor`, `graph.radius.rule`
Adaptive-radius graph controls passed to `dgraphs::create.rknn.graph()` when `graph = "rknn"`.

`transport.rule` Edge transport rule. Phase 1 implements `"procrustes"`.

`synchronize.orientation`
Logical. If `TRUE`, return deterministic spanning-tree orientation-synchronization metadata. Phase 1 does not mutate the returned frames.

`density.method` Sampling-density metadata rule. Phase 1 implements `"support.radius"`.

`alpha` Numeric exponent used only to report proposed future density-normalization weights.

`diagnostics` Logical. If `TRUE`, compute cycle diagnostics.

Details

The stored transport convention is column-vector based. For an oriented edge $i \leftarrow j$, `Oij` maps tangent coordinates from frame j into frame i:

$$v_j \mapsto O_{ij} v_j.$$

For shared-support Procrustes, row-coordinate matrices Z_i and Z_j are formed on the same vertex set. The row problem $\min_Q \|Z_j Q - Z_i\|_F^2$ gives $Q = UV^\top$ when $Z_j^\top Z_i = U\Sigma V^\top$. The stored column map is $O_{ij} = Q^\top = VU^\top$; the reported residual is $\|Z_j O_{ij}^\top - Z_i\|_F / \max(\|Z_i\|_F, \epsilon)$.

Value

A list of class `"pttf_geometry"`.

Examples

```
n <- 10L
X <- matrix(seq(0, 1, length.out = n), ncol = 1)
adj <- lapply(seq_len(n), function(i) intersect(c(i - 1L, i + 1L), 1:n))
lengths <- Map(function(i, j) abs(X[j, 1] - X[i, 1]), seq_len(n), adj)
pttf.geometry(X, adj, lengths, graph = "supplied", tangent.dim = 1L)
```

`pttf.operator` *Construct PTTF Transported-Difference Operators*

Description

Assembles experimental parallel-transport trend-filtering (PTTF) transported-difference operators from a `pttf.geometry` object. This is an operator-construction function only: it does not fit a response, tune a penalty parameter, or run an ℓ_1/ℓ_2 smoother.

Usage

```
pttf.operator(
  geometry,
  derivative.order = 3L,
  edge.status.policy = c("ok.only", "frame.fallback"),
 regression.weight.rule = c("inverse.length.squared", "inverse.length", "unit"),
  edge.length.epsilon = 1e-08,
  tensor.scaling = c("hs", "raw"),
  row.mass.rule = c("node.mass", "none"),
  row.normalize = c("none", "l2"),
  min.operator.rank.tol = 1e-10,
  max.operator.condition = 1e+08,
  return.intermediate = TRUE,
  return.A = TRUE,
  return.B = TRUE,
  diagnostics = TRUE
)
```

Arguments

`geometry`	A `"pttf_geometry"` object from `pttf.geometry`.
`derivative.order`	Integer derivative order, one of `1L`, `2L`, or `3L`.
`edge.status.policy`	Edge transport policy. `"ok.only"` uses only Phase 1 transports with status `"ok"`. `"frame.fallback"` also allows direct-frame fallback transports for non-OK shared-support statuses.
`regression.weight.rule`	Local regression edge-weight rule.
`edge.length.epsilon`	Positive numeric edge-length floor.
`tensor.scaling`	Symmetric tensor coordinate scaling. `"hs"` uses square-root multiplicity scaling so coordinate Euclidean norms match Hilbert–Schmidt norms. `"raw"` stores unscaled unique symmetric components.
`row.mass.rule`	Final row-mass multiplier. `"node.mass"` multiplies rows for vertex i by $\sqrt{\mu_i}$ from the Phase 1 density metadata. `"none"` leaves rows unweighted.

`row.normalize` Optional final row normalization.

`min.operator.rank.tol`
Relative singular-value tolerance for local derivative regression rank.

`max.operator.condition`
Maximum allowed weighted local-design condition number.

`return.intermediate`
Logical. If `TRUE`, include full logical intermediate derivative matrices.

`return.A` Logical. If `TRUE`, include the compact sparse row operator.

`return.B` Logical. If `TRUE`, include $A^\top A$.

`diagnostics` Logical. If `TRUE`, include assembly diagnostics.

Details

Phase 2 keeps a full logical vertex/component layout internally. For order r, the logical field has one block of $q_r = \binom{m+r-1}{r}$ components at each vertex. The returned `A` is compact: it includes rows only for accepted final-order vertex/component blocks, and `row.table$full.row` records the original full logical row.

For derivative level r, the local regression uses blocks $\Phi_r(u_{ij}) \in \mathbb{R}^{q_{r-1} \times q_r}$, lifted weights $W_i^{(r)} = \mathrm{diag}(w_{ij}) \otimes I_{q_{r-1}}$, and transported predecessor differences $K_{r-1}(O_{ij}) z_j - z_i$. Unavailable predecessor blocks are never filled with zero; affected neighbors are dropped and recorded.

Value

A list of class `"pttf_operator"` containing sparse operators, row/vertex provenance, tensor-basis metadata, and diagnostics.

Examples

```
n <- 10L
X <- matrix(seq(0, 1, length.out = n), ncol = 1)
adj <- lapply(seq_len(n), function(i) intersect(c(i - 1L, i + 1L), 1:n))
lengths <- Map(function(i, j) abs(X[j, 1] - X[i, 1]), seq_len(n), adj)
geometry <- pttf.geometry(
  X, adj, lengths, graph = "supplied", tangent.dim = 1L
)
pttf.operator(geometry, derivative.order = 2L)
```

---

pttf.operator.filter.rows

Filter Rows Of A PTTF Operator

Description

Creates a new `"pttf_operator"` object with a subset of compact operator rows. The sparse triplet payload is rebuilt from the filtered matrix so triplet row indices always refer to the filtered fit rows, while original compact and full logical row identities remain in `row.table`.

Usage

```
pttf.operator.filter.rows(
  operator,
  rows,
  reason = NULL,
  preserve.original = TRUE
)
```

Arguments

operator	A "pttf_operator" object from pttf.operator.
rows	Integer, logical, or character row selector. Character selectors are matched against row.table$status.
reason	Optional character reason stored in row.filter.
preserve.original	Logical. If TRUE, preserve original row identities in row.table$compact.row and row.table$full.row.

Value

A filtered "pttf_operator" object.

Examples

```
n <- 10L
X <- matrix(seq(0, 1, length.out = n), ncol = 1)
adj <- lapply(seq_len(n), function(i) intersect(c(i - 1L, i + 1L), 1:n))
lengths <- Map(function(i, j) abs(X[j, 1] - X[i, 1]), seq_len(n), adj)
geometry <- pttf.geometry(
  X, adj, lengths, graph = "supplied", tangent.dim = 1L
)
operator <- pttf.operator(geometry, derivative.order = 2L)
pttf.operator.filter.rows(operator, seq_len(max(1L, nrow(operator$A) - 2L)))
```

---

quadform.gradient *Evaluate gradients of all quadforms*

Description

Evaluate gradients of all quadforms

Usage

```
quadform.gradient(geometry, latent)
```

Arguments

geometry	A synthetic_quadform_geometry.
latent	Finite latent coordinates in rows.

Value

For one form, an n by d matrix. For multiple forms, an n by r by d array. With no forms, an n by zero by d array.

Examples

```
geometry <- synthetic.quadform(1L, 2L, forms = list(matrix(1)))
quadform.gradient(geometry, matrix(c(-1, 0, 1), ncol = 1))
```

---

quadform.metric *Evaluate the induced metric of a quadform geometry*

Description

Evaluate the induced metric of a quadform geometry

Usage

```
quadform.metric(geometry, latent)
```

Arguments

geometry	A synthetic_quadform_geometry.
latent	Finite latent coordinates in rows.

Value

For one row, a d by d matrix; otherwise an n by d by d array.

Examples

```
geometry <- synthetic.quadform(1L, 2L, forms = list(matrix(1)))
quadform.metric(geometry, matrix(c(0, 1), ncol = 1))
```

`refit.lpl.tf` *Refit A Local Polynomial Lifting Trend Filter*

Description

Reuses the fixed operator and selected lambda from an existing LPL-TF fit.

Usage

```
refit.lpl.tf(
  object,
  y,
  lambda = NULL,
  reuse.lambda = TRUE,
  verbose = FALSE,
  ...
)
```

Arguments

`object`	A `"lpl_tf"` object.
`y`	New numeric response vector.
`lambda`	Optional fixed lambda.
`reuse.lambda`	Logical. If `TRUE` and `lambda = NULL`, reuse `object$lambda`.
`verbose`	Logical.
`...`	Reserved.

Value

A refitted `"lpl_tf"` object.

Examples

```
if (requireNamespace("genlasso", quietly = TRUE)) {
  X <- matrix(seq(0, 1, length.out = 18), ncol = 1)
  fit <- fit.lpl.tf(X, X[, 1]^2, degree = 1L,
                    support.type = "knn", support.size = 7L,
                    lambda = 0.1, lambda.selection = "fixed")
  refit.lpl.tf(fit, y = X[, 1]^3)
}
```

`refit.malps` *Refit A MALPS Smoother With A New Response*

Description

Reuses the anchors, selected support profile, local supports, prediction supports, coordinate method, kernel, degree, and local-solver controls from a previous `fit.malps` result, then recomputes local polynomial coefficients for a new response vector. Observation weights, when supplied, multiply the stored geometric fitting weights for local coefficient estimation. Supports and model-averaging weights remain fixed. A weighted refit requires every stored local support to retain at least one positive effective fitting weight; sparse bootstrap-style weights can therefore fail even when the global weight vector is not all zero. If the original fit used robust local residual reweighting, robust weights are recomputed for the new response because they are response-dependent.

Usage

```
refit.malps(
  object,
  y = NULL,
  weights = NULL,
  reuse.selection = TRUE,
  refit.local.coefficients = TRUE,
  verbose = FALSE,
  ...
)
```

Arguments

`object`	A `"malps"` object from `fit.malps`.
`y`	Optional new numeric response vector with length `nrow(object$X)`. If `NULL`, the original response is reused.
`weights`	Optional nonnegative numeric observation weights with length `nrow(object$X)`. Zero weights remove observations from local coefficient estimation but do not change the stored supports or averaging weights. The refit fails if any local support has no positive effective fitting weight after multiplying by these observation weights.
`reuse.selection`	Currently requires `TRUE`.
`refit.local.coefficients`	Currently requires `TRUE`.
`verbose`	Logical; reserved for future progress messages.
`...`	Reserved for future extensions.

Value

A `"malps"` object with the same support profile and new fitted values.

Examples

```
X <- matrix(seq(0, 1, length.out = 20), ncol = 1)
fit <- fit.malps(X, X[, 1]^2, degree = 1L,
                 support.type = "knn", support.size = 8L)
refit.malps(fit, y = X[, 1]^3)
```

---

refit.metric.graph.lowpass

Refit Metric-Conductance Graph Low-Pass Regression

Description

Reuses a fitted metric graph low-pass eigensystem to smooth new responses.

Usage

```
refit.metric.graph.lowpass(
  fitted.model,
  y.new,
  per.column.gcv = FALSE,
  eta.grid = NULL,
  n.candidates = 40L,
  n.cores = 1L,
  block.size = NULL,
  verbose = FALSE
)
```

Arguments

`fitted.model`	A `"metric.graph.lowpass.fit"` object.
`y.new`	Numeric vector or matrix with one row per graph vertex.
`per.column.gcv`	Logical. If `TRUE`, select eta independently for each response column using the cached eigenbasis.
`eta.grid`	Optional positive numeric eta grid for per-column GCV.
`n.candidates`	Number of eta candidates when `eta.grid = NULL`.
`n.cores`	Number of cores for per-column GCV. Phase 1 uses sequential processing if optional parallel packages are unavailable.
`block.size`	Optional block size for fixed-eta multi-column refits.
`verbose`	Logical progress flag.

Value

A list of class `"metric.graph.lowpass.refit"`.

Examples

```
adj <- list(2L, c(1L, 3L), c(2L, 4L), 3L)
lengths <- list(1, c(1, 1), c(1, 1), 1)
fit <- fit.metric.graph.lowpass(
  adj, lengths, y = 1:4, n.eigenpairs = 4L,
  eta.grid = c(0.1, 1), eigen.solver = "dense"
)
refit.metric.graph.lowpass(fit, y.new = 4:1)
```

`refit.slpl.tf` *Refit A Fixed-Operator Synchronized LPL-TF Model*

Description

Refit A Fixed-Operator Synchronized LPL-TF Model

Usage

```
refit.slpl.tf(
  object,
  y,
  lambda1 = NULL,
  lambda2 = NULL,
  reuse.lambda = TRUE,
  verbose = FALSE,
  ...
)
```

Arguments

`object`	A `"slpl_tf"` fit.
`y`	New numeric response vector.
`lambda1`, `lambda2`	Optional fixed penalties. Defaults reuse `object$lambda1` and `object$lambda2`.
`reuse.lambda`	Logical. If `TRUE`, reuse omitted penalties.
`verbose`	Logical.
`...`	Reserved.

Value

A refitted `"slpl_tf"` object.

Examples

```
if (requireNamespace("genlasso", quietly = TRUE)) {
  X <- matrix(seq(0, 1, length.out = 18), ncol = 1)
  fit <- fit.slpl.tf(X, X[, 1]^2, degree = 1L,
                     support.type = "knn", support.size = 7L,
                     lambda1 = 0.1, lambda2 = 0,
                     lambda.selection = "fixed")
  refit.slpl.tf(fit, y = X[, 1]^3)
}
```

`refit.ssrhe.hessian.l1.regression`
Refit SSRHE-Style Hessian L1 Regression

Description

Reuses the A operator from `fit.ssrhe.hessian.l1.regression` to fit a new response or a new lambda grid without rebuilding local neighborhoods or local PCA Hessian rows.

Usage

```
refit.ssrhe.hessian.l1.regression(
  fitted.model,
  y.new = NULL,
  lambda.grid = fitted.model$lambda,
  lambda.selection = c("fixed", "cv"),
  weights = NULL,
  n.lambda = 40L,
  nfolds = 5L,
  fold.id = NULL,
  loss = c("mse", "mae"),
  selection = c("min", "one.se"),
  solver = c("genlasso", "admm", "auto"),
  row.scaling = c("none", "l2"),
  admm.rho = 1,
  admm.maxiter = 2000L,
  admm.abstol = 1e-04,
  admm.reltol = 0.001,
  maxsteps = 2000L,
  minlam = 0,
  approx = FALSE,
  rtol = 1e-07,
  btol = 1e-07,
  eps = 1e-04,
  verbose = FALSE
)
```

Arguments

`fitted.model`	A `"ssrhe.hessian.l1.fit"` object.
`y.new`	Optional new numeric response vector. If `NULL`, the original response is reused.
`lambda.grid`	Optional nonnegative lambda grid. For `lambda.selection = "fixed"`, this must contain exactly one value. For `lambda.selection = "cv"`, `NULL` builds a default grid from the fitted full-data generalized-lasso path.
`lambda.selection`	`"cv"` for observed-label K-fold cross-validation or `"fixed"` for a supplied fixed lambda.
`weights`	Optional nonnegative observation weights. Missing responses automatically receive zero weight.
`n.lambda`	Number of default lambda candidates when `lambda.grid = NULL` and `lambda.selection = "cv"`.
`nfolds`	Number of validation folds over observed positive-weight labels. Ignored when `fold.id` is supplied.
`fold.id`	Optional integer fold assignments of length `nrow(X)`.
`loss`	Validation loss, currently `"mse"` or `"mae"`.
`selection`	Selection rule. `"min"` chooses the smallest mean validation loss. `"one.se"` chooses the largest lambda within one standard error of the minimum.
`solver`	Solver backend. `"genlasso"` uses the generalized-lasso path backend. `"admm"` uses a fixed-lambda ADMM solver for each lambda value. `"auto"` tries `"genlasso"` first and falls back to ADMM when path extraction produces an error or non-finite fitted values.
`row.scaling`	Optional row scaling for the penalty matrix before solving. `"l2"` scales nonzero rows of A to unit Euclidean norm.
`admm.rho`, `admm.maxiter`, `admm.abstol`, `admm.reltol`	ADMM controls used when `solver = "admm"` or when `solver = "auto"` falls back to ADMM.
`maxsteps`, `minlam`, `approx`, `rtol`, `btol`, `eps`, `verbose`	Controls passed to **genlasso**.

Value

A list of class `"ssrhe.hessian.l1.refit"`.

Examples

```
X <- matrix(seq(0, 1, length.out = 12), ncol = 1)
fit <- fit.ssrhe.hessian.l1.regression(
  X, X[, 1]^2, k = 6L, tangent.dim = 1L,
  lambda.grid = 0.05, lambda.selection = "fixed", solver = "admm"
)
refit.ssrhe.hessian.l1.regression(
  fit, y.new = X[, 1]^3, solver = "admm"
)
```

`refit.ssrhe.hessian.regression` *Refit SSRHE-Style Hessian-Energy Regression*

Description

Reuses the operator from `fit.ssrhe.hessian.regression` to fit new responses or new fixed penalty weights without rebuilding local PCA neighborhoods or Hessian-energy matrices.

Usage

```
refit.ssrhe.hessian.regression(
  fitted.model,
  y.new = NULL,
  lambda1 = fitted.model$lambda$lambda1,
  lambda2 = fitted.model$lambda$lambda2,
  weights = NULL,
  ridge = fitted.model$lambda$ridge,
  verbose = FALSE
)
```

Arguments

`fitted.model`	A `"ssrhe.hessian.fit"` object.
`y.new`	New numeric response vector or matrix with one row per vertex. If `NULL`, the original response is reused.
`lambda1`	Nonnegative Hessian-energy penalty multiplier for $f^\top Bf = \|Af\|_2^2$.
`lambda2`	Nonnegative supplemental-stabilizer multiplier for $f^\top B_S f$. If positive, `stabilizer` must be `TRUE`. Currently supported only for `derivative.order = 2L`.
`weights`	Optional nonnegative observation weights. May be `NULL`, a vector of length `nrow(X)`, or a matrix with the same dimensions as `y`.
`ridge`	Nonnegative diagonal ridge added to the linear system for numerical stabilization.
`verbose`	Logical. If `TRUE`, print a short native construction message.

Value

A list of class `"ssrhe.hessian.refit"`.

Examples

```
X <- matrix(seq(0, 1, length.out = 12), ncol = 1)
fit <- fit.ssrhe.hessian.regression(
  X, X[, 1]^2, k = 6L, tangent.dim = 1L, lambda1 = 0.1
)
refit.ssrhe.hessian.regression(fit, y.new = X[, 1]^3)
```

`slpl.tf.operator` *Construct A Synchronized LPL-TF Fixed Operator*

Description

Builds the fixed S-LPL-TF operator pair. The LPL component A_{LPL} is the accepted self-excluded LPL-TF residual operator from `lpl.tf.operator`. The synchronization component C_{sync} compares inclusive local polynomial prediction maps over overlapping supports.

Usage

```
slpl.tf.operator(
  X,
  adj.list = NULL,
  weight.list = NULL,
  graph = NULL,
  graph.stage = "final",
  anchor.index = NULL,
  anchor.coordinates = NULL,
  degree = 2L,
  support.type = c("adaptive.radius", "knn", "fixed.radius"),
  support.size = NULL,
  radius = NULL,
  min.support = NULL,
  support.buffer = 3L,
  kernel = c("epanechnikov", "triangular", "gaussian", "tricube"),
  coordinate.method = c("coordinates", "local.pca"),
  chart.dim = NULL,
  support.metric = c("auto", "coordinates", "graph.geodesic"),
  auto.chart.support.metric = c("coordinates", "operator", "both"),
  auto.chart.selection.metric = c("coordinates", "operator"),
  row.normalize = c("l2", "none", "l1"),
  local.solver = c("auto", "normal.equations", "qr", "svd"),
  normal.equations.max.condition = 1e+08,
  duplicate.action = c("keep", "error"),
  drop.rank.deficient = TRUE,
  sync.row.normalize = c("l2"),
  sync.min.norm = 1e-12,
  verbose = FALSE,
  ...
)
```

Arguments

`X`	Numeric coordinate matrix with one row per observation.

adj.list, weight.list
: Optional supplied undirected graph adjacency and positive edge-length lists using 1-based vertex indices.

graph
: Optional graph object returned by dgraphs::create.rknn.graph() or a list containing adj.list/weight.list or adj_list/weight_list.

graph.stage
: Graph stage to extract from graph: "final", "raw", or "pruned".

anchor.index
: Optional integer vector of observed anchor/target indices. The current implementation supports observed anchors only.

anchor.coordinates
: Reserved for later off-observation anchors; this implementation requires NULL.

degree
: Polynomial degree. The current implementation supports 0L, 1L, and 2L.

support.type
: Coordinate support rule. "knn" uses the nearest support.size candidates including the target before self exclusion. "adaptive.radius" uses the nearest min.support positive predictors after self exclusion. "fixed.radius" uses all points within radius.

support.size
: Positive integer for support.type = "knn".

radius
: Positive coordinate radius for support.type = "fixed.radius".

min.support
: Minimum number of positive-weight predictors after self exclusion. If NULL, uses choose(ncol(X) + degree, degree) + support.buffer.

support.buffer
: Nonnegative integer added to the local polynomial design size when choosing default supports.

kernel
: Kernel used to weight local predictors by distance.

coordinate.method
: Coordinate chart used for the local polynomial design. "coordinates" uses centered ambient coordinates; "local.pca" uses a deterministic local PCA chart on the selected support.

chart.dim
: Chart dimension. For "coordinates", this must be NULL or ncol(X). For "local.pca", NULL defaults to ncol(X). The special value "auto" estimates a single chart dimension from observed-coordinate local PCA spectra only, without using responses, truth values, latent coordinates, or labels.

support.metric
: Support-distance rule. "coordinates" uses Euclidean coordinate distances; "graph.geodesic" uses shortest-path distances in the supplied graph. "auto" uses graph geodesics when a graph is supplied and coordinate distances otherwise.

auto.chart.support.metric
: Support system used when chart.dim = "auto". "coordinates" uses Euclidean coordinate neighborhoods, "operator" uses the resolved operator support metric, and "both" computes both diagnostics side by side.

auto.chart.selection.metric
: Which auto chart-dimension diagnostic to use for the fitted operator when auto.chart.support.metric = "both". The default "coordinates" preserves historical behavior.

row.normalize
: Complete-row normalization rule applied after setting target coefficient +1 and predictor coefficients -h_ij.

local.solver
: Local linear algebra rule.

`normal.equations.max.condition`
: Maximum condition number for `local.solver = "auto"` to use normal equations.

`duplicate.action`
: Duplicate coordinate policy.

`drop.rank.deficient`
: Logical. The current implementation requires `TRUE`.

`sync.row.normalize`
: Synchronization-row normalization. Phase S2 uses `"l2"` by default.

`sync.min.norm`
: Minimum raw synchronization-row norm. Rows below this threshold are dropped with metadata.

`verbose`
: Logical. Reserved for diagnostic messages.

`...`
: Reserved.

Value

A list of class `"slpl_tf_operator"` containing `A_LPL`, `C_sync`, row metadata, diagnostics, settings, and the embedded `"lpl_tf_operator"`.

Examples

```
X <- matrix(seq(0, 1, length.out = 18), ncol = 1)
slpl.tf.operator(X, degree = 1L, support.type = "knn",
                 support.size = 7L, kernel = "gaussian")
```

---

ssrhe.hessian.operator

Construct an SSRHE-Style Local Hessian Energy Operator

Description

Constructs the discrete local Hessian operator used by the semi-supervised regularization framework of Kim, Steinke, and Hein (2009). The constructor is intended as a package-facing, auditable R/C++ port of the reference behavior: it returns the sparse row operator A, the quadratic energy matrix $B = A^\top A$, and optionally the supplemental stabilizer B_S.

Usage

```
ssrhe.hessian.operator(
  X,
  k = NULL,
  tangent.dim,
  nn.index = NULL,
  neighborhood.type = c("knn", "adaptive.radius", "supplied"),
  support.index = NULL,
  adaptive.k.scale = NULL,
```

```
  radius.rule = c("geomean", "max", "min"),
  radius.factor = 1.25,
  min.support = NULL,
  max.support = NULL,
  support.buffer = 2L,
  support.topup = c("nearest", "none"),
  tangent.dim.rule = c("fixed", "eigen.cumulative"),
  eigen.tolerance = 0.95,
  derivative.order = 2L,
  stabilizer = FALSE,
  pinv.tol = sqrt(.Machine$double.eps),
  local.solver = c("auto", "normal.equations", "svd", "qr"),
  normal.equations.max.condition = 10000,
  return.A = TRUE,
  return.B = TRUE,
  return.BS = stabilizer,
  return.sparse = TRUE,
  return.local.diagnostics = TRUE,
  return.timing = FALSE,
  verbose = FALSE
)
```

Arguments

X	Numeric matrix with one observation per row. Distances for the default neighborhood search are Euclidean distances in these coordinates.
k	Integer number of nearest neighbors per point, including the point itself, used when neighborhood.type = "knn". This follows the SSRHE Matlab convention. For adaptive-radius neighborhoods, k may be omitted when adaptive.k.scale is supplied.
tangent.dim	Integer tangent dimension used for the local PCA chart. Required when tangent.dim.rule = "fixed". If NULL and tangent.dim.rule = "eigen.cumulative", the dimension is selected locally from the PCA variance ratio.
nn.index	Optional integer matrix of neighbor indices, with nrow(X) rows and k columns. Each row must contain its center vertex. If NULL, Euclidean k-NN including self is computed in C++.
neighborhood.type	Local support rule. "knn" uses the original rectangular self-including kNN neighborhoods. "adaptive.radius" builds variable-size supports from dgraphs::create.rknn.graph "supplied" uses support.index directly.
support.index	Optional list of integer vectors, one per row of X. Each element gives a variable-size local support and must contain its center vertex.
adaptive.k.scale	Integer local-scale k used by dgraphs::create.rknn.graph() when neighborhood.type = "adaptive.radius".
radius.rule, radius.factor	Adaptive-radius graph parameters passed to dgraphs::create.rknn.graph().

`min.support` Optional minimum local support size for adaptive-radius supports. Defaults to the local quadratic design size plus `support.buffer`, clamped to `nrow(X)`.

`max.support` Optional maximum local support size. Oversized adaptive supports are trimmed to the closest `max.support` vertices while keeping the center vertex.

`support.buffer` Nonnegative integer added to the local quadratic design size when choosing the default `min.support`.

`support.topup` How undersized adaptive-radius supports are enlarged. `"nearest"` appends ambient nearest neighbors. `"none"` leaves supports unchanged and lets the C++ operator reject undersized supports.

`tangent.dim.rule`
Either `"fixed"` or `"eigen.cumulative"`.

`eigen.tolerance`
Cumulative local PCA variance threshold used when `tangent.dim.rule = "eigen.cumulative"` and `tangent.dim = NULL`.

`derivative.order`
Integer derivative order of the local SSRHE-style operator. `2L` is the original local Hessian energy. `3L` is an experimental third-derivative energy whose rows estimate unique symmetric third-derivative tensor components with factorial and tensor-multiplicity scaling.

`stabilizer` Logical. If `TRUE`, also construct the supplemental stabilizer matrix described in the SSRHE supplement. Currently supported only for `derivative.order = 2L`.

`pinv.tol` Nonnegative tolerance multiplier for local pseudoinverses.

`local.solver` Local least-squares backend used to map local function values to derivative coefficients. `"auto"` is the default: it uses normal equations when the local design is full rank and has condition number no larger than `normal.equations.max.condition`, and otherwise falls back to SVD. `"normal.equations"` requests the normal-equation solve for full-rank local designs and falls back only on hard numerical failures. `"svd"` is the most stable reference path. `"qr"` uses pivoted QR and falls back to SVD for rank-deficient local designs.

`normal.equations.max.condition`
Positive condition-number guard used by `local.solver = "auto"` before accepting the normal-equation backend. The default is deliberately conservative because normal-equation solves square the effective condition number and order-3 near-minimum local supports can be numerically fragile.

`return.A` Logical. If `TRUE`, return A as a sparse matrix.

`return.B` Logical. If `TRUE`, return $B = A^\top A$.

`return.BS` Logical. If `TRUE` and `stabilizer = TRUE`, return the supplemental stabilizer B_S.

`return.sparse` Logical. If `TRUE`, attach **Matrix** sparse matrices in addition to raw triplets.

`return.local.diagnostics`
Logical. If `TRUE`, compute additional R-side local chart diagnostics such as chart distortion and boundary asymmetry. These diagnostics are useful for operator audits, but can be skipped in fitting and cross-validation paths for speed.

`return.timing` Logical. If `TRUE`, attach a phase-level elapsed time table to the returned operator. The timings separate R-side validation, neighborhood/support construction,

native local operator construction, optional local diagnostics, sparse matrix assembly, and output finalization. For adaptive-radius neighborhoods, subphase timings are also attached in `neighborhoods$timing`.

`verbose` Logical. If `TRUE`, print a short native construction message.

Details

For each point x_i, the operator constructs a local PCA chart from a self-including local support, projects the support into $\mathbb{R}^m$, and centers the local coordinates at x_i. A local quadratic model is then fitted with the intercept fixed at f_i:

$$f(x_j) - f(x_i) \approx \sum_{a \le b} h_{ab} z_{ja} z_{jb} + \sum_a g_a z_{ja}.$$

The local linear map from function values to the quadratic coefficients is the Matlab-compatible

$$\mathrm{RegMat} = X^+ - X^+ \mathrm{IndMat},$$

where X is the reduced quadratic-plus-linear design and IndMat copies the center value into all local rows. Diagonal Hessian components are scaled by $\sqrt{2}$ and off-diagonal components by 1, so that the row energy matches the reference Hessian energy. With `derivative.order = 3L`, the reduced local design uses cubic monomials first, followed by quadratic and linear monomials. The returned rows estimate unique symmetric third-derivative components $\partial_{abc} f$ with scale

$$s_{abc} = m_{abc} \sqrt{\mu_{abc}},$$

where m_{abc} is the factorial monomial-to-derivative multiplier (6 for aaa, 2 for aab, and 1 for three distinct indices) and μ_{abc} is the ordered-tensor multiplicity (1, 3, or 6). Thus $\|Af\|_2^2$ approximates the squared Frobenius norm of the full symmetric third-derivative tensor.

The returned A is the stacked sparse matrix of these local derivative coefficient rows. The ℓ_2 SSRHE penalty is

$$f^\top B f = \|Af\|_2^2, \quad B = A^\top A.$$

Exposing A is useful for auditability and for future ℓ_1-style variants based on $\|Af\|_1$.

Adaptive-radius graph construction uses **dgraphs**; fixed-k and supplied neighborhoods are package-local geosmooth paths.

Value

A list of class `"ssrhe.hessian.operator"` containing:

- `A`: sparse local Hessian row operator, if requested;
- `B`: sparse quadratic energy matrix $A^\top A$, if requested;
- `BS`: optional supplemental stabilizer matrix;
- `A.triplet`, `BS.triplet`: raw sparse triplets;
- `nn.index`: neighbor index matrix for rectangular kNN neighborhoods, if used;
- `support.index`: list of actual local supports used by the backend;
- `neighborhoods`: support-construction diagnostics;

- `row.table`: one row per Hessian component row of A;
- `diagnostics`: local design rank, condition, and PCA summaries;
- `local.diagnostics`: if requested, one row per center vertex with support size, design rank/condition, PCA variance, chart-distortion, boundary-asymmetry, and curvature-bias proxy diagnostics;
- `timing`: if requested, a phase-level elapsed-time table;
- `native.timing`: if requested, a C++ backend subphase timing table for native operator construction;
- `parity`: notes documenting reference-behavior conventions.

References

Kim, K. I., Steinke, F., and Hein, M. (2009). Semi-supervised regression using Hessian energy with an application to semi-supervised dimensionality reduction. *Advances in Neural Information Processing Systems 22*. https://papers.nips.cc/paper_files/paper/2009/hash/f4552671f8909587cf485ea990207f3b-Abstract.html

Examples

```
X <- matrix(seq(0, 1, length.out = 12), ncol = 1)
ssrhe.hessian.operator(X, k = 6L, tangent.dim = 1L)
```

`ssrhe.support.grid` *Build Candidate Support Profiles for SSRHE Adaptive-Radius Tuning*

Description

Constructs a compact grid of adaptive-radius support profiles for use with `support.selection = "cv"` in SSRHE fitting functions. Each row gives an `adaptive.k.scale` value and a requested `min.support`. The grid is intentionally small by default because support selection nests operator construction inside response cross-validation.

Usage

```
ssrhe.support.grid(
  n,
  tangent.dim,
  derivative.order = 2L,
  support.buffer = 2L,
  max.candidates = 8L
)
```

Arguments

n	Number of observations.
tangent.dim	Tangent dimension used by the SSRHE local polynomial design.
derivative.order	SSRHE derivative order, currently 2L or 3L.
support.buffer	Nonnegative integer added to the local design size when constructing the smallest candidate support.
max.candidates	Maximum number of candidate support profiles to return.

Value

A data frame with columns adaptive.k.scale, min.support, and max.support. max.support is NA by default, meaning no truncation.

Examples

```
ssrhe.support.grid(n = 50L, tangent.dim = 2L, max.candidates = 4L)
```

---

summary.harmonic_smoother

Summary Method for Harmonic Smoother Results

Description

Provides detailed summary statistics for harmonic smoother results, including the evolution of extrema counts and basin structure differences.

Usage

```
## S3 method for class 'harmonic_smoother'
summary(object, ...)
```

Arguments

object	An object of class "harmonic_smoother".
...	Further arguments passed to or from other methods.

Value

An object of class "summary.harmonic_smoother" containing:

stable_iteration	The iteration at which topology stabilized
iterations_recorded	Total number of recorded iterations

`initial_extrema`
: Number of extrema at the first iteration

`initial_maxima`
: Number of maxima at the first iteration

`initial_minima`
: Number of minima at the first iteration

`final_extrema`
: Number of extrema at the final iteration

`final_maxima`
: Number of maxima at the final iteration

`final_minima`
: Number of minima at the final iteration

`extrema_reduction`
: Reduction in number of extrema

`topology_diff_summary`
: Summary statistics of topology differences

See Also

`harmonic.smoother`, `print.summary.harmonic_smoother`

`synthetic.circle` *Specify a circle geometry*

Description

Specify a circle geometry

Usage

```
synthetic.circle(
  radius = 1,
  angle.range = c(0, 2 * pi),
  ambient.dim = 2L,
  frame = c("canonical", "random.orthonormal", "supplied"),
  frame.algorithm = NULL,
  frame.matrix = NULL,
  offset = NULL
)
```

Arguments

`radius`
: Circle radius.

`angle.range`
: Admissible angular interval.

`ambient.dim`
: Ambient dimension.

`frame`, `frame.algorithm`, `frame.matrix`, `offset`
: Frame parameters.

Value

A synthetic geometry component.

Examples

```
synthetic.circle(radius = 2, angle.range = c(0, pi))
```

---

synthetic.dataset.checksum *Compute the canonical content checksum of a synthetic dataset*

Description

Compute the canonical content checksum of a synthetic dataset

Usage

```
synthetic.dataset.checksum(x)
```

Arguments

x	A synthetic_dataset.

Value

A lowercase SHA-256 string.

Examples

```
x <- materialize.synthetic(synthetic.registry.spec("G1"), n = 20L, seed = 1L)
synthetic.dataset.checksum(x)
```

---

synthetic.helix *Specify a helix geometry*

Description

Specify a helix geometry

Usage

```
synthetic.helix(
  pitch = 0.2,
  t.range = c(0, 2 * pi),
  ambient.dim = 3L,
  frame = c("canonical", "random.orthonormal", "supplied"),
  frame.algorithm = NULL,
  frame.matrix = NULL,
  offset = NULL
)
```

Arguments

pitch	Helix pitch.
t.range	Admissible parameter interval.
ambient.dim	Ambient dimension.
frame, frame.algorithm, frame.matrix, offset	Frame parameters.

Value

A synthetic geometry component.

Examples

```
synthetic.helix(pitch = 0.25, t.range = c(0, pi))
```

---

synthetic.point.line.junction

Specify a point-line junction

Description

Specify a point-line junction

Usage

```
synthetic.point.line.junction(
  point.location,
  line.origin,
  line.direction,
  line.range
)
```

Arguments

point.location	Point location.
line.origin, line.direction, line.range	Segment parameters.

Value

A two-stratum synthetic_stratified_geometry.

Examples

```
synthetic.point.line.junction(c(0, 0), c(0, 0), c(1, 0), c(0, 1))
```

`synthetic.quadform` *Specify a quadform geometry*

Description

Specify a quadform geometry

Usage

```
synthetic.quadform(
  intrinsic.dim,
  ambient.dim,
  forms = list(),
  frame = c("canonical", "random.orthonormal", "supplied"),
  frame.algorithm = NULL,
  frame.matrix = NULL,
  offset = NULL
)
```

Arguments

`intrinsic.dim`	Intrinsic dimension.
`ambient.dim`	Ambient dimension.
`forms`	List of finite symmetric quadratic-form matrices.
`frame`	Frame policy.
`frame.algorithm`	Versioned random-frame algorithm or `NULL`.
`frame.matrix`	Supplied orthonormal frame or `NULL`.
`offset`	Ambient offset or `NULL`.

Value

A synthetic geometry component.

Examples

```
synthetic.quadform(1L, 2L, forms = list(matrix(0.5)))
```

synthetic.registry.ids

List maintained synthetic recipe IDs

Description

List maintained synthetic recipe IDs

Usage

```
synthetic.registry.ids()
```

Value

Character recipe IDs.

Examples

```
head(synthetic.registry.ids())
```

synthetic.registry.seed

Resolve the legacy seed for an SSRHE registry recipe

Description

Resolve the legacy seed for an SSRHE registry recipe

Usage

```
synthetic.registry.seed(
  recipe.id,
  replicate = 1L,
  n = NULL,
  base.seed = 273001L
)
```

Arguments

recipe.id	A one-dimensional, flat, or quadform SSRHE recipe ID.
replicate	Positive replicate number.
n	Sample size. Required for flat and quadform recipes.
base.seed	One-dimensional suite base seed.

Value

A validated integer seed.

Examples

```
synthetic.registry.seed("S16.V1", replicate = 2L)
```

`synthetic.registry.spec`

Resolve a maintained synthetic recipe

Description

Default recipes are reconstructed from normalized component foreign keys. Parameter overrides are accepted only for the legacy G-family compatibility surface and remain content-bound, non-frozen specifications.

Usage

```
synthetic.registry.spec(recipe.id, parameters = list())
```

Arguments

`recipe.id`	One of `synthetic.registry.ids()`.
`parameters`	Optional named parameter overrides.

Value

A validated `synthetic_spec`.

Examples

```
synthetic.registry.spec("G1")
```

synthetic.response.bernoulli *Bernoulli response specification*

Description

Bernoulli response specification

Usage

```
synthetic.response.bernoulli(minimum.positive = 0L, maximum.attempts = 1L)
```

Arguments

minimum.positive	Minimum accepted positive responses.
maximum.attempts	Maximum complete redraw attempts.

Value

A synthetic response component.

Examples

```
synthetic.response.bernoulli(minimum.positive = 1L, maximum.attempts = 5L)
```

synthetic.response.clustered.gaussian *Clustered Gaussian response specification*

Description

Clustered Gaussian response specification

Usage

```
synthetic.response.clustered.gaussian(residual.sd, intraclass.correlation)
```

Arguments

residual.sd	Residual standard deviation.
intraclass.correlation	Intraclass correlation in [0,1).

Value

A synthetic response component.

Examples

```
synthetic.response.clustered.gaussian(0.2, 0.3)
```

---

synthetic.response.gaussian
Gaussian response specification

Description

Gaussian response specification

Usage

```
synthetic.response.gaussian(sd)
```

Arguments

sd	Response standard deviation.

Value

A synthetic response component.

Examples

```
synthetic.response.gaussian(sd = 0.2)
```

---

synthetic.response.heteroskedastic.gaussian
Heteroskedastic Gaussian response specification

Description

Heteroskedastic Gaussian response specification

Usage

```
synthetic.response.heteroskedastic.gaussian(base.sd, truth.multiplier)
```

Arguments

base.sd	Base standard deviation.
truth.multiplier	Multiplier applied to truth.

Value

A synthetic response component.

Examples

```
synthetic.response.heteroskedastic.gaussian(0.1, 0.2)
```

---

synthetic.response.laplace.outlier

Laplace response with Gaussian contamination

Description

Laplace response with Gaussian contamination

Usage

```
synthetic.response.laplace.outlier(
  laplace.scale,
  outlier.fraction,
  outlier.sd,
  minimum.outliers = 0L,
  count.rounding = "round",
  laplace.algorithm = "uniform.inverse.v1"
)
```

Arguments

laplace.scale	Laplace scale.
outlier.fraction	Fraction contaminated.
outlier.sd	Contamination standard deviation.
minimum.outliers	Minimum contamination count.
count.rounding	Count policy.
laplace.algorithm	Versioned Laplace algorithm.

Value

A synthetic response component.

Examples

```
synthetic.response.laplace.outlier(0.1, 0.05, 1)
```

`synthetic.sampling.clustered` *Clustered sampling specification*

Description

Clustered sampling specification

Usage

```
synthetic.sampling.clustered(
  cluster.count,
  observations.per.cluster,
  center.lower = -1,
  center.upper = 1,
  within.sd,
  algorithm = "centers.then.gaussian.offsets.v1"
)
```

Arguments

`cluster.count`	Number of clusters.
`observations.per.cluster`	Rows per cluster.
`center.lower, center.upper`	Center box bounds.
`within.sd`	Within-cluster standard deviation.
`algorithm`	Versioned draw algorithm.

Value

A fixed-size synthetic sampling component.

Examples

```
synthetic.sampling.clustered(3L, 5L, within.sd = 0.1)
```

`synthetic.sampling.dirichlet.zeros` *Dirichlet sampling with structural zeros*

Description

Dirichlet sampling with structural zeros

Usage

```
synthetic.sampling.dirichlet.zeros(
  concentration,
  zero.fraction,
  zero.parts,
  zero.row.policy = c("first", "random"),
  count.rounding = "round",
  algorithm = "normalized.gamma.v1"
)
```

Arguments

`concentration`	Scalar or part-wise Dirichlet concentration.
`zero.fraction`	Fraction of rows receiving structural zeros.
`zero.parts`	Part indices set to zero.
`zero.row.policy`	Row-selection policy.
`count.rounding`	Count rule.
`algorithm`	Versioned draw algorithm.

Value

A synthetic sampling component.

Examples

```
synthetic.sampling.dirichlet.zeros(
  concentration = rep(1, 3), zero.fraction = 0.2, zero.parts = 1L
)
```

`synthetic.sampling.gapped.uniform` *Gapped-uniform sampling specification*

Description

Gapped-uniform sampling specification

Usage

```
synthetic.sampling.gapped.uniform(
  intervals,
  allocation = c("multinomial", "fixed.proportion", "fixed.count"),
  probabilities = NULL,
  counts = NULL,
  rounding = c("largest.remainder", "floor.first.remainder.last"),
  order = c("draw", "ascending"),
  algorithm = "sequential.interval.runif.v1"
)
```

Arguments

`intervals`	Two-column matrix of disjoint intervals.
`allocation`	Allocation policy.
`probabilities`	Optional allocation probabilities.
`counts`	Optional fixed counts.
`rounding`	Fixed-proportion rounding rule.
`order`	Ordering policy.
`algorithm`	Versioned draw algorithm.

Value

A synthetic sampling component.

Examples

```
intervals <- rbind(c(-1, -0.25), c(0.25, 1))
synthetic.sampling.gapped.uniform(intervals, probabilities = c(0.5, 0.5))
```

synthetic.sampling.grid.interval

Deterministic interval-grid sampling specification

Description

Deterministic interval-grid sampling specification

Usage

```
synthetic.sampling.grid.interval(
  lower,
  upper,
  endpoints = c("exclude.lower", "exclude.upper", "include.both")
)
```

Arguments

lower, upper	Interval bounds.
endpoints	Endpoint convention. "exclude.lower" reproduces the historical circle grid; "include.both" reproduces the historical uniform trefoil grid.

Value

A deterministic synthetic sampling component.

Examples

```
synthetic.sampling.grid.interval(0, 2 * pi, endpoints = "exclude.lower")
```

synthetic.sampling.stratified

Legacy G4 stratified sampling specification

Description

Legacy G4 stratified sampling specification

Usage

```
synthetic.sampling.stratified(
  fraction.a = 0.5,
  algorithm = c("stratum.sequential.v1", "legacy.g4.stratum.sequential.v1")
)
```

Arguments

`fraction.a`	Fraction allocated to stratum A.
`algorithm`	Versioned traversal algorithm.

Value

A synthetic sampling component.

Examples

```
synthetic.sampling.stratified(fraction.a = 0.6)
```

`synthetic.sampling.truncated.normal` *Truncated-normal sampling specification*

Description

Truncated-normal sampling specification

Usage

```
synthetic.sampling.truncated.normal(
  mean,
  sd,
  lower,
  upper,
  order = c("draw", "ascending"),
  algorithm = "inverse.cdf.v1"
)
```

Arguments

`mean`, `sd`	Normal parameters.
`lower`, `upper`	Truncation bounds.
`order`	Ordering policy.
`algorithm`	Versioned draw algorithm.

Value

A synthetic sampling component.

Examples

```
synthetic.sampling.truncated.normal(0, 1, -2, 2)
```

synthetic.sampling.uniform.box

Uniform-box sampling specification

Description

Uniform-box sampling specification

Usage

```
synthetic.sampling.uniform.box(
  lower,
  upper,
  order = c("draw", "ascending.first.coordinate"),
  algorithm = "column.major.runif.v1"
)
```

Arguments

lower, upper	Scalar or coordinate-wise bounds.
order	Row ordering policy.
algorithm	Versioned draw algorithm.

Value

A synthetic sampling component.

Examples

```
synthetic.sampling.uniform.box(lower = c(-1, 0), upper = c(1, 2))
```

synthetic.sampling.uniform.disk

Uniform-disk sampling specification

Description

Uniform-disk sampling specification

Usage

```
synthetic.sampling.uniform.disk(radius = 1, algorithm = "radial.sqrt.v1")
```

Arguments

radius	Disk radius.
algorithm	Versioned draw algorithm.

Value

A synthetic sampling component.

Examples

```
synthetic.sampling.uniform.disk(radius = 2)
```

---

synthetic.sampling.uniform.interval

Uniform-interval sampling specification

Description

Uniform-interval sampling specification

Usage

```
synthetic.sampling.uniform.interval(
  lower,
  upper,
  order = c("draw", "ascending"),
  algorithm = "runif.v1"
)
```

Arguments

lower, upper	Interval bounds.
order	Ordering policy.
algorithm	Versioned draw algorithm.

Value

A synthetic sampling component.

Examples

```
synthetic.sampling.uniform.interval(0, 1, order = "ascending")
```

synthetic.sampling.uniform.rectangle *Uniform-rectangle sampling specification*

Description

Uniform-rectangle sampling specification

Usage

```
synthetic.sampling.uniform.rectangle(
  lower,
  upper,
  algorithm = "coordinate.sequential.runif.v1"
)
```

Arguments

lower, upper	Length-two coordinate bounds.
algorithm	Versioned draw algorithm.

Value

A synthetic sampling component.

Examples

```
synthetic.sampling.uniform.rectangle(c(-1, -2), c(1, 2))
```

synthetic.simplex *Specify a simplex geometry*

Description

Specify a simplex geometry

Usage

```
synthetic.simplex(parts)
```

Arguments

parts	Number of compositional parts.

Value

A synthetic geometry component.

Examples

```
synthetic.simplex(parts = 3L)
```

`synthetic.spec` *Assemble a synthetic-data specification*

Description

Combines draw-free geometry, sampling, truth, and response components into one canonically hashable specification.

Usage

```
synthetic.spec(
  geometry,
  sampling,
  truth,
  response,
  recipe.id = NULL,
  registry.tag = NULL,
  compatibility = NULL,
  metadata = list()
)
```

Arguments

`geometry`	A synthetic geometry component.
`sampling`	A synthetic sampling component.
`truth`	A synthetic truth component.
`response`	A synthetic response component.
`recipe.id`	Optional readable recipe label.
`registry.tag`	Optional stable experimental-plan tag.
`compatibility`	Optional serializable legacy compatibility metadata.
`metadata`	Optional serializable scientific metadata.

Value

A `synthetic_spec`.

Examples

```
spec <- synthetic.spec(
  synthetic.circle(), synthetic.sampling.uniform.interval(0, 2 * pi),
  synthetic.truth.named("helix.sin.v1"), synthetic.response.gaussian(0.1)
)
spec$specification.sha256
```

synthetic.sphere.cap *Specify a sphere-cap geometry*

Description

Specify a sphere-cap geometry

Usage

```
synthetic.sphere.cap(
  radius = 2,
  footprint.radius = 1,
  ambient.dim = 3L,
  frame = c("canonical", "random.orthonormal", "supplied"),
  frame.algorithm = NULL,
  frame.matrix = NULL,
  offset = NULL
)
```

Arguments

`radius`	Sphere radius.
`footprint.radius`	Radius of the planar cap footprint.
`ambient.dim`	Ambient dimension.
`frame`, `frame.algorithm`, `frame.matrix`, `offset`	Frame parameters.

Value

A synthetic geometry component.

Examples

```
synthetic.sphere.cap(radius = 2, footprint.radius = 1)
```

synthetic.stratified *Assemble a stratified geometry*

Description

Assemble a stratified geometry

Usage

```
synthetic.stratified(strata, junctions = NULL)
```

Arguments

strata	Nonempty list of compatible synthetic_stratum objects.
junctions	Optional data frame describing stratum boundary junctions.

Value

A draw-free synthetic geometry component.

Examples

```
point <- synthetic.stratum.point("point", c(0, 0))
line <- synthetic.stratum.segment("line", c(0, 1), c(0, 0), c(1, 0))
synthetic.stratified(list(point, line))
```

---

synthetic.stratum.point

Specify a point stratum

Description

Specify a point stratum

Usage

```
synthetic.stratum.point(id, location)
```

Arguments

id	Stable stratum identifier.
location	Finite ambient location.

Value

A draw-free synthetic_stratum.

Examples

```
synthetic.stratum.point("origin", c(0, 0))
```

synthetic.stratum.rectangle

Specify a rectangle stratum

Description

Specify a rectangle stratum

Usage

```
synthetic.stratum.rectangle(id, coordinate.ranges, origin, basis)
```

Arguments

`id`	Stable stratum identifier.
`coordinate.ranges`	Two-row matrix of finite increasing ranges.
`origin`	Finite ambient origin.
`basis`	Orthonormal ambient-by-two basis.

Value

A draw-free `synthetic_stratum`.

Examples

```
synthetic.stratum.rectangle(
  "square", rbind(c(-1, 1), c(-1, 1)), c(0, 0), diag(2)
)
```

synthetic.stratum.segment

Specify a line-segment stratum

Description

Specify a line-segment stratum

Usage

```
synthetic.stratum.segment(id, coordinate.range, origin, direction)
```

Arguments

`id`	Stable stratum identifier.
`coordinate.range`	Finite increasing intrinsic range.
`origin`	Finite ambient origin.
`direction`	Unit ambient direction.

Value

A draw-free `synthetic_stratum`.

Examples

```
synthetic.stratum.segment("line", c(-1, 1), c(0, 0), c(1, 0))
```

`synthetic.torus.patch` *Specify a torus-patch geometry*

Description

Specify a torus-patch geometry

Usage

```
synthetic.torus.patch(
  major.radius = 1,
  minor.radius = 0.35,
  u.range = c(-pi/2, pi/2),
  v.range = c(-pi/2, pi/2),
  ambient.dim = 3L,
  frame = c("canonical", "random.orthonormal", "supplied"),
  frame.algorithm = NULL,
  frame.matrix = NULL,
  offset = NULL
)
```

Arguments

`major.radius`, `minor.radius`	Torus radii.
`u.range`, `v.range`	Admissible angular intervals.
`ambient.dim`	Ambient dimension.
`frame`, `frame.algorithm`, `frame.matrix`, `offset`	Frame parameters.

Value

A synthetic geometry component.

Examples

```
synthetic.torus.patch(major.radius = 2, minor.radius = 0.5)
```

`synthetic.trefoil` *Specify a trefoil-knot geometry*

Description

This preserves the legacy `gflow` parameterization: `x = scale * sin(t) + 2 * sin(2*t)`, `y = scale * cos(t) - 2 * cos(2*t)`, and `z = -scale * sin(3*t)`.

Usage

```
synthetic.trefoil(
  scale = 1,
  t.range = c(0, 2 * pi),
  ambient.dim = 3L,
  frame = c("canonical", "random.orthonormal", "supplied"),
  frame.algorithm = NULL,
  frame.matrix = NULL,
  offset = NULL
)
```

Arguments

`scale`	Scale applied to the first harmonic and third coordinate.
`t.range`	Admissible parameter interval.
`ambient.dim`	Ambient dimension.
`frame`, `frame.algorithm`, `frame.matrix`, `offset`	Frame parameters.

Value

A synthetic geometry component.

Examples

```
synthetic.trefoil(scale = 0.5, t.range = c(0, pi))
```

`synthetic.truth.gaussian.mixture` *Specify a Gaussian-mixture truth*

Description

Specify a Gaussian-mixture truth

Usage

```
synthetic.truth.gaussian.mixture(
  centers,
  scales,
  weights,
  normalize = c("none", "sample.max"),
  evaluation.coordinates = "latent"
)
```

Arguments

`centers`	Component centers, one per row.
`scales`	Positive isotropic standard deviations or covariance matrices.
`weights`	Nonnegative mixture weights.
`normalize`	Normalization scope.
`evaluation.coordinates`	Coordinates on which to evaluate.

Value

A synthetic truth component.

Examples

```
synthetic.truth.gaussian.mixture(
  centers = rbind(-1, 1), scales = c(0.5, 0.5), weights = c(1, 1)
)
```

synthetic.truth.logit *Specify a sinusoidal finite-design logit truth*

Description

Specify a sinusoidal finite-design logit truth

Usage

```
synthetic.truth.logit(
  amplitude = 1.5,
  target.prevalence = 0.5,
  clip = c(0.05, 0.95)
)
```

Arguments

amplitude	Sinusoidal log-odds amplitude.
target.prevalence	Target mean pre-clipping probability.
clip	Probability bounds.

Value

A synthetic truth component.

Examples

```
synthetic.truth.logit(amplitude = 1, target.prevalence = 0.4)
```

synthetic.truth.named *Specify a versioned named truth evaluator*

Description

Specify a versioned named truth evaluator

Usage

```
synthetic.truth.named(id, parameters = list())
```

Arguments

id	Evaluator ID.
parameters	Serializable evaluator parameters.

Value

A synthetic truth component.

Examples

```
synthetic.truth.named("intrinsic.linear.first.v1")
```

`synthetic.truth.occupation.mixture`
Specify a finite-design occupation-mixture truth

Description

The analytic Gaussian-mixture density is transformed to Bernoulli occupation probabilities by `probability.maximum * density^gamma / max(density^gamma)`.

Usage

```
synthetic.truth.occupation.mixture(
  centers,
  covariances,
  weights,
  gamma = 1,
  probability.maximum = 0.65,
  normalization = "design.maximum"
)
```

Arguments

`centers`	Component centers, one per row.
`covariances`	Positive-definite covariance matrices.
`weights`	Nonnegative mixture weights.
`gamma`	Positive density-shape exponent.
`probability.maximum`	Maximum realized occupation probability.
`normalization`	Currently `"design.maximum"`.

Value

A finite-design synthetic truth component.

Examples

```
synthetic.truth.occupation.mixture(
  centers = rbind(c(-1, 0), c(1, 0)),
  covariances = list(diag(2), diag(2)), weights = c(1, 1)
)
```

synthetic.truth.polynomial

Specify a polynomial truth

Description

Specify a polynomial truth

Usage

```
synthetic.truth.polynomial(coefficients, evaluation.coordinates = "latent")
```

Arguments

coefficients	Named polynomial coefficients.
evaluation.coordinates	Coordinates on which to evaluate.

Value

A synthetic truth component.

Examples

```
synthetic.truth.polynomial(c(b0 = 1, b1 = 2, b11 = -0.5))
```

transported.graph.hessian.operator

Construct a Transported Graph Hessian Operator

Description

Builds an experimental transported-Hessian graph operator without fitting a response. This is the phase-0 through phase-2 diagnostic layer for the transported graph Hessian trend-filtering project: it constructs directed edge differences, matches directions across a base dart, assembles a second- or third-difference diagnostic operator, and returns diagnostics that make the transport rule auditable.

Usage

```
transported.graph.hessian.operator(
  adj.list,
  weight.list = NULL,
  transport.order = 2L,
 transport.rule = c("exact.coordinate", "local.embedding.soft", "edge.angle.hard",
    "edge.angle.soft", "regression.gradient"),
```

```
  coordinates = NULL,
  direction.labels = NULL,
  polynomial.probes = NULL,
 local.embedding.method = c("auto", "coordinates", "grip.edge.kk", "mds.edge.kk",
    "cmdscale"),
  local.embedding.dim = 2L,
  local.disk.hops = 1L,
  local.max.vertices = 50L,
  return.sparse = TRUE,
  tol = 1e-08,
  soft.angle.scale = NULL,
  soft.length.scale = NULL,
  soft.bandwidth = 0.25,
  max.match.angle = NULL,
  max.length.relative.error = NULL,
  min.match.margin = NULL,
  max.effective.matches = NULL,
 match.threshold.rule = c("none", "fixed", "local.quantile", "local.robust.z"),
  match.score.quantile = 0.25,
  match.margin.quantile = 0.5,
  min.best.score.z = 1,
  min.margin.z = 0,
  max.effective.match.fraction = NULL,
  edge.angle.scale = NULL,
  edge.length.scale = NULL,
  edge.angle.bandwidth = 0.35,
  edge.angle.max.angle.difference = NULL,
  edge.angle.max.length.relative.error = NULL,
  gradient.coordinate.method = c("coordinates", "local.embedding"),
  gradient.embedding.method = c("grip.edge.kk", "mds.edge.kk", "cmdscale"),
  gradient.embedding.dim = NULL,
  gradient.disk.hops = local.disk.hops,
  gradient.max.vertices = local.max.vertices,
 gradient.disk.rule = c("hops", "metric.diameter.fraction", "metric.local.scale"),
  gradient.disk.radius.fraction = 0.1,
 gradient.disk.local.scale.method = c("knn.distance", "median.incident.length",
    "quantile.incident.length"),
  gradient.disk.local.scale.k = 8L,
  gradient.disk.local.scale.quantile = 0.75,
  gradient.disk.local.scale.multiplier = 2,
  gradient.disk.min.vertices = 0L,
  gradient.chart.selection = c("fixed", "adaptive"),
  gradient.embedding.candidates = c("cmdscale", "mds.edge.kk"),
  gradient.disk.rule.candidates = c("hops", "metric.diameter.fraction",
    "metric.local.scale"),
  gradient.disk.hops.candidates = 1:5,
  gradient.disk.radius.fraction.candidates = c(0.05, 0.075, 0.1, 0.15, 0.2),
  gradient.disk.local.scale.multiplier.candidates = c(1, 1.5, 2, 3, 4),
```

```
  gradient.ridge = 1e-08,
  gradient.quadratic.disk.hops = 2L,
  gradient.quadratic.max.vertices = gradient.max.vertices
)
```

Arguments

`adj.list`	List of integer neighbor vectors using 1-based vertex indices. The graph must be undirected.
`weight.list`	Optional list of positive edge lengths parallel to `adj.list`. If `NULL`, all edge lengths are one.
`transport.order`	Integer scalar, either `2L` or `3L`. `2L` constructs the transported Hessian-like second-difference operator. `3L` currently constructs a supplied-coordinate regression-quadratic third-difference operator and is supported only for `transport.rule = "regression.gradient"` with `gradient.coordinate.method = "coordinates"`.
`transport.rule`	Character scalar. `"exact.coordinate"` uses exact direction labels. `"local.embedding.soft"` uses coordinate direction vectors and softmax transport weights. `"edge.angle.hard"` and `"edge.angle.soft"` use coordinate-derived edge angles relative to the base dart. `"regression.gradient"` compares locally estimated gradient components.
`coordinates`	Optional numeric matrix with one row per vertex. For `transport.rule = "exact.coordinate"`, coordinates must define axis-aligned graph edges so direction labels can be inferred. Coordinates are required by `"edge.angle.hard"` and `"edge.angle.soft"`.
`direction.labels`	Optional list parallel to `adj.list`; each entry gives the exact direction label for the corresponding outgoing dart. When supplied, these labels override labels inferred from `coordinates`.
`polynomial.probes`	Optional numeric vector or matrix with one row per vertex. If supplied, residual diagnostics $\|AP\|_F/\|P\|_F$ are reported for the transported Hessian matrix A.
`local.embedding.method`	Character scalar controlling the coordinates used by `transport.rule = "local.embedding.soft"`. `"auto"` uses supplied `coordinates` when available and otherwise tries `"grip.edge.kk"`. `"coordinates"` uses supplied coordinates directly. `"grip.edge.kk"` builds a local graph disk and prefers weighted GRIP followed by true edge-KK optimization when the installed **grip** exposes `weighted.grip()` and `edge.kk()`. Older compatibility names are used only as fallbacks. `"mds.edge.kk"` uses classical MDS followed by the same edge-KK optimizer when available. `"cmdscale"` uses classical MDS only.
`local.embedding.dim`	Positive integer embedding dimension for local graph-disk embeddings.
`local.disk.hops`	Non-negative integer hop radius around each base dart used by graph-derived local embedding methods.
`local.max.vertices`	Positive integer cap on local disk size. If a disk is larger, the nearest vertices by hop distance are retained.

`return.sparse` Logical. If `TRUE`, attach **Matrix** sparse matrices to the returned payloads.

`tol` Positive numeric tolerance for coordinate-axis direction inference.

`soft.angle.scale`, `soft.length.scale`
Optional positive numeric scales for the soft transport angular and length score components. If `NULL`, robust global defaults are estimated from candidate dart comparisons.

`soft.bandwidth` Positive numeric softmax bandwidth τ. Smaller values make the soft rule closer to hard nearest-direction matching.

`max.match.angle`
Optional non-negative numeric angle threshold in radians. For soft transport, candidate Hessian rows whose best match has angle larger than this threshold are dropped.

`max.length.relative.error`
Optional non-negative numeric threshold for the best match's relative edge-length error, $|\ell_{\mathrm{matched}} - \ell_{\mathrm{direction}}|/\ell_{\mathrm{direction}}$. Candidate rows above the threshold are dropped.

`min.match.margin`
Optional non-negative numeric threshold for the difference between the second-best and best soft-match scores. Candidate rows with smaller margins are dropped.

`max.effective.matches`
Optional positive numeric threshold for $\exp(H)$, where H is the softmax transport entropy. Candidate rows with more diffuse matches are dropped.

`match.threshold.rule`
Character scalar. `"none"` and `"fixed"` apply only the explicit fixed gates above. `"local.quantile"` also gates rows by local candidate-score and margin quantiles. `"local.robust.z"` also gates rows by robust local z-scores for best-match score and margin.

`match.score.quantile`, `match.margin.quantile`
Quantile thresholds used by `match.threshold.rule = "local.quantile"`. The best score must lie at or below `match.score.quantile`; the best-vs-second margin must lie at or above `match.margin.quantile`.

`min.best.score.z`, `min.margin.z`
Non-negative robust-z thresholds used by `match.threshold.rule = "local.robust.z"`. A larger best-score z-score means the best candidate is unusually low-scoring relative to local alternatives. A larger margin z-score means the best-vs-second separation is unusually large.

`max.effective.match.fraction`
Optional positive numeric threshold for $\exp(H)/n_{\mathrm{candidate}}$. Candidate rows whose softmax mass is too diffuse across the local target directions are dropped.

`edge.angle.scale`, `edge.length.scale`
Optional positive numeric scales for edge-angle matching. If `NULL`, robust global medians are estimated from candidate angle differences and length differences.

`edge.angle.bandwidth`
Positive numeric softmax bandwidth used only by `transport.rule = "edge.angle.soft"`.

`edge.angle.max.angle.difference`
Optional non-negative threshold, in radians, for accepting an edge-angle match.

edge.angle.max.length.relative.error
: Optional non-negative threshold for accepting an edge-angle match based on relative edge-length error.

gradient.coordinate.method
: Character scalar used only by transport.rule = "regression.gradient". "coordinates" uses the supplied global coordinates. "local.embedding" estimates the two endpoint gradients of each base dart in one shared graph-derived local chart.

gradient.embedding.method
: Character scalar used by gradient.coordinate.method = "local.embedding". The choices match the graph-derived local embedding backends used by local.embedding.soft.

gradient.embedding.dim
: Optional positive integer dimension for graph-derived regression-gradient local charts. If NULL, the supplied coordinate dimension is used when available, otherwise local.embedding.dim.

gradient.disk.hops
: Non-negative integer hop radius for graph-derived regression-gradient local charts.

gradient.max.vertices
: Positive integer cap on graph-derived regression-gradient local chart size.

gradient.disk.rule
: Character scalar controlling graph-derived regression-gradient disk construction. "hops" uses gradient.disk.hops. "metric.diameter.fraction" uses a two-center graph-geodesic disk whose metric radius is gradient.disk.radius.fraction times the graph diameter. "metric.local.scale" uses a two-center graph-geodesic disk whose metric radius is gradient.disk.local.scale.multiplier times the larger endpoint local scale.

gradient.disk.radius.fraction
: Positive numeric scalar used by gradient.disk.rule = "metric.diameter.fraction".

gradient.disk.local.scale.method
: Character scalar controlling the per-vertex metric scale used by gradient.disk.rule = "metric.local.scale". "knn.distance" uses the weighted graph distance to the gradient.disk.local.scale.k-th nearest vertex. "median.incident.length" and "quantile.incident.length" use incident edge-length summaries.

gradient.disk.local.scale.k
: Positive integer neighborhood index used by gradient.disk.local.scale.method = "knn.distance".

gradient.disk.local.scale.quantile
: Numeric probability in [0, 1] used by gradient.disk.local.scale.method = "quantile.incident.length".

gradient.disk.local.scale.multiplier
: Positive numeric scalar multiplier for gradient.disk.rule = "metric.local.scale".

gradient.disk.min.vertices
: Non-negative integer lower target for metric disk coverage. Metric disks whose radius selects too few vertices are expanded to include at least this many nearest vertices, subject to gradient.max.vertices.

gradient.chart.selection
: Character scalar used only by graph-derived regression-gradient transport. "fixed" uses gradient.embedding.method and gradient.disk.hops. "adaptive"

tries `gradient.embedding.candidates` crossed with `gradient.disk.hops.candidates` for each base dart and chooses the chart with the lowest graph-only diagnostic score.

`gradient.embedding.candidates`
: Character vector of graph-derived local embedding backends considered by `gradient.chart.selection = "adaptive"`.

`gradient.disk.rule.candidates`
: Character vector of disk construction rules considered by `gradient.chart.selection = "adaptive"`.

`gradient.disk.hops.candidates`
: Non-negative integer vector of hop radii considered by `gradient.chart.selection = "adaptive"`.

`gradient.disk.radius.fraction.candidates`
: Positive numeric vector of graph-diameter fractions considered by `gradient.chart.selection = "adaptive"`.

`gradient.disk.local.scale.multiplier.candidates`
: Positive numeric vector of local-scale multipliers considered by `gradient.chart.selection = "adaptive"`.

`gradient.ridge`
: Non-negative ridge parameter used by `transport.rule = "regression.gradient"` when inverting local weighted least-squares normal equations.

`gradient.quadratic.disk.hops`
: Non-negative integer hop radius for the supplied-coordinate local quadratic regressions used by `transport.order = 3L`.

`gradient.quadratic.max.vertices`
: Positive integer cap on local quadratic-regression disk size for `transport.order = 3L`.

Details

For a dart $u \to v$, the first difference is

$$\delta_{u \to v} f = \frac{f(v) - f(u)}{\ell_{uv}}.$$

For a base dart $u \to u'$ and a matched outgoing direction $u \to v \leftrightarrow u' \to v'$, the transported Hessian row is

$$\delta_{u' \to v'} f - \delta_{u \to v}.$$

The reference rule, `transport.rule = "exact.coordinate"`, matches directions with identical coordinate labels. Labels may be supplied directly through `direction.labels`, or inferred from axis-aligned `coordinates`. The first general metric rule, `transport.rule = "local.embedding.soft"`, uses supplied coordinates to softly match directions by angle and edge length. The edge-angle rules, `"edge.angle.hard"` and `"edge.angle.soft"`, match directions by comparing their angle relative to the transported base edge. `transport.rule = "regression.gradient"` estimates local least-squares gradients and compares gradient components across graph darts. Those gradients can be computed either from supplied coordinates or from a graph-derived local embedding built in a shared disk around each base dart.

Value

A list of class "transported.graph.hessian.operator" with the canonical graph, directed-edge table, first-difference matrix, transported Hessian matrix, row metadata, dropped candidate rows, and diagnostics. For graph-derived regression-gradient transport with supplied coordinates, the embedding diagnostics also include synthetic chart-quality checks against those ambient coordinates.

Examples

```
adj <- list(2L, c(1L, 3L), c(2L, 4L), 3L)
weights <- list(1, c(1, 1), c(1, 1), 1)
x <- 0:3
transported.graph.hessian.operator(
  adj, weights, coordinates = matrix(x, ncol = 1),
  polynomial.probes = cbind(1, x, x^2)
)
```

---

validate.synthetic.dataset

Validate a canonical synthetic dataset

Description

Validate a canonical synthetic dataset

Usage

```
validate.synthetic.dataset(x)
```

Arguments

x	A synthetic_dataset.

Value

x, invisibly.

Examples

```
x <- materialize.synthetic(synthetic.registry.spec("G1"), n = 20L, seed = 1L)
validate.synthetic.dataset(x)
```

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