

Package ‘ISPAT3D’

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Type Package

Title Spatial Conditional Association Networks in Registered Tumor Volumes

Version 0.3.1

Description Fits tumor-zone-specific conditional cell-density networks from registered three-dimensional multiplex imaging. An anisotropic Matern-3/2 Gaussian process is estimated per variable and zone using a Vecchia likelihood on spatially balanced anchors; predictions at all selected cells yield residual covariance sufficient statistics. Gaussian maximum likelihood then fits a shared-plus-zone factor covariance model. A matched section-wise planar fit uses the same selected cells and covariance estimator. This extends the spatially informed cell-density analysis of Bhadury et al. (2026) [doi:10.1038/s41598-026-35341-8](https://doi.org/10.1038/s41598-026-35341-8).

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Imports gpboost, graphics, stats, utils

Suggests data.table, knitr, rmarkdown, testthat (>= 3.0.0)

VignetteBuilder knitr

URL <https://github.com/sagnikbhadury/ISPAT-3D>

BugReports <https://github.com/sagnikbhadury/ISPAT-3D/issues>

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Author Sagnik Bhadury [aut, cre]

Maintainer Sagnik Bhadury <bhadury@umich.edu>

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ispat3d_edge_table	<i>Extract signed conditional-association edges</i>
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Description

Uses partial correlations from a full fitted zone covariance. A low-rank shared factor covariance alone is not invertible and is not a network input.

Usage

```
ispat3d_edge_table(x, zone = NULL, threshold = 0)
```

Arguments

- x An ISPAT3D fit returned by ispat3d_fit() or a partial-correlation matrix.
- zone Zone name when x is a fit.
- threshold Minimum absolute partial correlation to retain.

Value

A data frame with source, target, effect, sign, and magnitude, sorted by decreasing absolute effect.

ispat3d_example_image *Simulate a small registered cell map with section-wise KDE inputs*

Description

Generates a didactic cell map with three annotated cell types, section-wise Gaussian kernel-density estimates evaluated at every cell, and two relative tumor-density zones per section. It is designed for package examples and checks, not for biological simulation studies.

Usage

```
ispat3d_example_image(
  n_per_section = 24L,
  n_sections = 3L,
  bandwidth = 0.12,
  seed = 2026L
)
```

Arguments

n_per_section	Cells per section; an even multiple of six, at least 24.
n_sections	Number of serial sections, at least two.
bandwidth	Gaussian KDE bandwidth in the simulated coordinate units.
seed	Reproducible simulation seed.

Value

A list containing coordinates, sections, source cell types, KDE values, transformed model matrix Y, zones, and tumor-density score.

ispat3d_fit *Fit current ISPAT-3D on selected cells*

Description

Fits a Mat rn-3/2 anisotropic GP per variable and zone using a 15-neighbor Vecchia likelihood on spatially balanced anchors; predicts at all selected cells; then fits shared-plus-zone covariance from complete residual covariance summaries by Gaussian maximum likelihood.

Usage

```
ispat3d_fit(
  Y,
  coords,
  zones,
  sections = rep(1L, nrow(Y)),
  rank = 5L,
  anchor_fraction = 0.1,
  anchor_min = 300L,
  anchor_max = 5000L,
  neighbors = 15L,
  gp_maxit = 30L,
  factor_maxit = 350L,
  seed = 2026L,
  threads = 2L,
  return_residuals = FALSE
)
```

Arguments

<code>Y</code>	Numeric cells-by-variables matrix, usually $\log 1p(1e9 * KDE)$.
<code>coords</code>	Numeric cells-by-3 matrix in registered x,y,z coordinates.
<code>zones</code>	Zone label for each row.
<code>sections</code>	Section identifier for balanced anchor selection.
<code>rank</code>	Shared and zone-specific factor rank (default 5).
<code>anchor_fraction</code>	Fraction of cells selected as GP anchors.
<code>anchor_min, anchor_max</code>	Minimum and maximum number of anchors per fit.
<code>neighbors</code>	Number of Vecchia neighbors.
<code>gp_maxit</code>	Maximum GP likelihood iterations.
<code>factor_maxit</code>	Maximum covariance likelihood iterations.
<code>seed</code>	Random seed for anchor selection and GP fits.
<code>threads</code>	GPBoost threads per GP fit.
<code>return_residuals</code>	Whether to return full adjusted residual matrices.

Value

List containing shared covariance, full zone covariances, zone partial correlations, diagnostics, and optionally residuals.

ispat3d_fit_2d

*Fit the matched section-wise ISPAT-2D comparator***Description**

Uses the same selected rows and covariance estimator as ispat3d_fit(), but fits independent planar GPs within each zone-section group. Groups with fewer than 10 cells are mean-centered; failed planar GP fits are recorded and mean-centered. This changes both spatial dimension and section pooling.

Usage

```
ispat3d_fit_2d(
  Y,
  coords,
  zones,
  sections,
  rank = 5L,
  anchor_fraction = 0.1,
  anchor_min = 300L,
  anchor_max = 5000L,
  neighbors = 15L,
  gp_maxit = 30L,
  factor_maxit = 350L,
  seed = 2026L,
  threads = 2L,
  return_residuals = FALSE
)
```

Arguments

Y	Numeric cells-by-variables matrix, usually log1p(1e9 * KDE).
coords	Numeric cells-by-3 matrix in registered x,y,z coordinates.
zones	Zone label for each row.
sections	Required section identifier for every selected cell.
rank	Shared and zone-specific factor rank (default 5).
anchor_fraction	Fraction of cells selected as GP anchors.
anchor_min, anchor_max	Minimum and maximum number of anchors per fit.
neighbors	Number of Vecchia neighbors.
gp_maxit	Maximum GP likelihood iterations.
factor_maxit	Maximum covariance likelihood iterations.
seed	Random seed for anchor selection and GP fits.

threads GPBoost threads per GP fit.

return_residuals Whether to return full adjusted residual matrices.

Value

Same structure as ispat3d_fit().

ispat3d_fit_covariance	<i>Fit shared and zone-specific factor covariance from sufficient statistics</i>
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Description

Fits $\Sigma_q = \Phi \Phi' + \Lambda_q \Lambda_q' + \text{diag}(\psi_q)$ by a weighted Gaussian covariance likelihood. This is the current estimator used after Vecchia GP adjustment, not a variational factor posterior.

Usage

ispat3d_fit_covariance(covariances, counts, rank = 5L, maxit = 350L)

Arguments

covariances Named list of complete sample covariance matrices.

counts Number of adjusted cells in each zone, in list order.

rank Shared and zone-specific loading rank (default 5).

maxit Maximum L-BFGS-B iterations.

Value

Shared covariance, full zone covariances, partial correlations, loadings, uniquenesses, and optimization diagnostics.

`ispat3d_partial_correlation`*Convert a full covariance matrix to partial correlations*

Description

Convert a full covariance matrix to partial correlations

Usage

```
ispat3d_partial_correlation(covariance, ridge = 1e-06)
```

Arguments

<code>covariance</code>	Symmetric positive-definite covariance matrix.
<code>ridge</code>	Small numerical diagonal ridge (default 1e-6).

Value

A signed partial-correlation matrix.

`ispat3d_plot_network` *Plot a circular partial-correlation network using base graphics*

Description

The fitted zone covariance is transformed to partial correlations using the full shared, zone-specific, and uniqueness terms. Red and blue edges show positive and negative conditional density associations.

Usage

```
ispat3d_plot_network(  
  x,  
  zone = NULL,  
  threshold = 0.05,  
  main = zone,  
  positive = "#B2182B",  
  negative = "#2166AC",  
  vertex_cex = 1.1,  
  label_cex = 0.75,  
  edge_scale = 4  
)
```

Arguments

<code>x</code>	An ISPAT3D fit or partial-correlation matrix.
<code>zone</code>	Zone name when <code>x</code> is a fit.
<code>threshold</code>	Minimum absolute partial correlation to display.
<code>main</code>	Plot title.
<code>positive, negative</code>	Edge colors for positive and negative associations.
<code>vertex_cex</code>	Node size multiplier.
<code>label_cex</code>	Label size multiplier.
<code>edge_scale</code>	Controls edge widths.

Value

Invisibly returns the displayed edge table.

<code>ispat3d_plot_zones</code>	<i>Facet all fitted zone networks in one base-R figure</i>
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Description

Facet all fitted zone networks in one base-R figure

Usage

```
ispat3d_plot_zones(fit, zones = names(fit$full), columns = 2L, ...)
```

Arguments

<code>fit</code>	An ISPAT3D fit from <code>ispat3d_fit()</code> or <code>ispat3d_fit_2d()</code> .
<code>zones</code>	Zone names to plot, in order.
<code>columns</code>	Number of panel columns.
<code>...</code>	Further arguments passed to <code>ispat3d_plot_network()</code> .

Value

Invisibly returns a named list of displayed edge tables.

ispat3d_sample	<i>Select spatially balanced cells by zone and section</i>
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Description

Select spatially balanced cells by zone and section

Usage

```
ispat3d_sample(  
  coords,  
  zones,  
  sections,  
  budget,  
  budget_kind = c("per_zone", "total"),  
  seed = 2026L  
)
```

Arguments

coords	N-by-3 registered coordinate matrix.
zones	Zone label per row.
sections	Section identifier per row.
budget	Number per zone when budget_kind="per_zone"; total otherwise.
budget_kind	One of "per_zone" or "total".
seed	Sampling seed.

Value

Named list of source row indices for each zone.

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