Package 'SingRegKrig'

August 8, 2026

Type Package

Title Singularity Regression Kriging for Spatial Prediction

Version 0.1.0

Description Implements the Singularity Regression Kriging ('SRK') model for spatial prediction by integrating covariate singularity feature construction, nonlinear trend estimation via random forest, and geostatistical interpolation of residuals using ordinary kriging. Singularity-based anomaly indices are computed from environmental covariates at multiple spatial scales to capture local multiscale heterogeneity and augment the random forest feature set for trend estimation. The resulting residuals are interpolated using ordinary kriging to generate final spatial predictions with uncertainty quantification. Tools for spatial block cross-validation, parameter sensitivity analysis, and diagnostic visualization are also provided. Methods are based on Ren, Song, Chen, and Yu (2026) <doi:10.1080/15481603.2026.2690341>, with singularity theory from Cheng (2012) <doi:10.1016/j.gexplo.2012.07.007> and Cheng (2017) <doi:10.1016/j.gr.2017.07.011>, random forest methodology from Breiman (2001) <doi:10.1023/A:1010933404324>, and regression kriging framework from Hengl, Heuvelink, and Rossiter (2007) <doi:10.1016/j.cageo.2007.05.001>.

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Encoding UTF-8

RoxygenNote 7.3.3

Depends R (>= 4.0.0)

Imports stats, graphics, grDevices, randomForest, gstat, sp

Suggests testthat (>= 3.0.0)

LazyData true

NeedsCompilation no

Author Shikhar Tyagi [aut, cre] (ORCID: <https://orcid.org/0000-0003-1606-0844>),
Arvind Pandey [aut],

Bhupendra Singh [aut],
Vrijesh Tripathi [aut]

Maintainer Shikhar Tyagi <shikhar1093tyagi@gmail.com>

Repository CRAN

Date/Publication 2026-08-08 12:30:18 UTC

Contents

`compute_singularity` *Compute Singularity Indices for Spatial Covariates*

Description

Computes singularity-based anomaly indices from environmental covariates at multiple spatial scales. For each location, the singularity index characterises how the local covariate intensity changes with spatial scale, following the singularity theory of Cheng (2012, 2017).

Usage

```
compute_singularity(
  coords,
  values,
  scales = NULL,
  min_neighbours = 3L,
  min_scales = 2L
)
```

Arguments

- `coords` A numeric matrix or data frame with two columns representing spatial coordinates (e.g., easting and northing). Coordinate units must match the units used in `scales`.
- `values` A numeric vector of covariate values at the locations specified by `coords`. Must have the same length as the number of rows in `coords`.
- `scales` A numeric vector of spatial scales at which to compute the singularity index. Scales should be positive and in the same units as `coords`. If `NULL`, defaults to 10 equally spaced scales spanning one-tenth to one-half of the coordinate range.
- `min_neighbours` Integer. Minimum number of valid neighbouring samples required within a scale window for that scale to be used. Default is 3.
- `min_scales` Integer. Minimum number of valid scales required to estimate the singularity index at a location. Locations with fewer valid scales are assigned the neutral value of 2. Default is 2.

Details

The singularity index is computed following the method described in Ren et al. (2026) and based on the singularity theory of Cheng (2012, 2017, 2018). For each location s and spatial scale r, the local covariate intensity $C(A(s,r))$ is estimated as the mean of the absolute covariate values within a square window of half-width r centred at s. The singularity index $\alpha(s)$ is then estimated as the slope of the ordinary least-squares regression of $\log C$ on $\log r$, plus 2:

$$\alpha(s) = \hat{\beta}_1(s) + 2$$

where $\hat{\beta}_1(s)$ is the OLS slope from regressing $\log C(A(s,r))$ on $\log r$ across the selected scales. A value of $\alpha = 2$ corresponds to a spatially uniform field; $\alpha < 2$ indicates local enrichment; $\alpha > 2$ indicates local depletion.

Value

A numeric vector of singularity indices with the same length as the number of rows in `coords`. A value of 2 indicates a spatially uniform field (neutral reference); values less than 2 indicate local enrichment (positive anomaly); values greater than 2 indicate local depletion.

References

Cheng, Q. (2012). Singularity theory and methods for mapping geochemical anomalies caused by buried sources and for predicting undiscovered mineral deposits in covered areas. *Journal of Geochemical Exploration*, **122**, 55–70. doi:10.1016/j.gexplo.2012.07.007

Cheng, Q. (2017). Singularity analysis of global zircon U-Pb age series and implication of continental crust evolution. *Gondwana Research*, **51**, 51–63. doi:10.1016/j.gr.2017.07.011

Ren, K., Song, Y., Chen, M., and Yu, Q. (2026). A singularity regression kriging for spatial prediction. *GIScience & Remote Sensing*, **63**(1), 2690341. doi:10.1080/15481603.2026.2690341

Examples

```
set.seed(42)
coords <- as.matrix(expand.grid(x = 1:10, y = 1:10))
values <- rnorm(100)
alpha <- compute_singularity(coords, values, scales = c(1, 2, 3, 4, 5))
summary(alpha)

# Uniform field returns singularity = 2
alpha_uniform <- compute_singularity(coords, rep(1, 100),
                                      scales = c(1, 2, 3, 4, 5))
all(abs(alpha_uniform - 2) < 1e-10)
```

---

plot.srk — *Plot Diagnostics for an SRK Model*

Description

Produces diagnostic plots for a fitted SRK model, including residual histogram, variable importance, observed vs fitted, and variogram plots.

Usage

```
## S3 method for class 'srk'
plot(x, which = c(1L, 2L, 3L, 4L), ...)
```

Arguments

`x`	An object of class "`srk`".
`which`	Integer vector specifying which plots to produce. 1 = residual histogram, 2 = variable importance, 3 = observed vs fitted, 4 = variogram. Default is `c(1, 2, 3, 4)`.
`...`	Additional arguments passed to plotting functions.

Value

Invisibly returns `NULL`.

Examples

```
sim_data <- sim_srk_data(n_side = 10, scenario = "normal", seed = 42)
model <- srk(z ~ cov1, data = sim_data, coords = ~x + y,
             scales = c(1, 2, 3, 4, 5), ntree = 100)
plot(model, which = 3)
```

plot.srk_cv *Plot Cross-Validation Results*

Description

Produces an observed vs predicted scatter plot from spatial block cross-validation.

Usage

```
## S3 method for class 'srk_cv'
plot(x, ...)
```

Arguments

`x`	An object of class `"srk_cv"`.
`...`	Additional arguments passed to `plot`.

Value

Invisibly returns `NULL`.

plot.srk_sensitivity *Plot Sensitivity Analysis Results*

Description

Produces a heatmap of performance metrics across parameter combinations.

Usage

```
## S3 method for class 'srk_sensitivity'
plot(x, metric = "R2", ...)
```

Arguments

`x`	An object of class `"srk_sensitivity"`.
`metric`	Character. Metric to plot. One of `"R2"`, `"RMSE"`, or `"MAE"`. Default is `"R2"`.
`...`	Additional arguments passed to `image`.

Value

Invisibly returns `NULL`.

`predict.srk` *Predict from a Singularity Regression Kriging Model*

Description

Generates spatial predictions at new locations using a fitted SRK model. Computes singularity features at prediction locations, evaluates the random forest trend, and performs ordinary kriging of residuals.

Usage

```
## S3 method for class 'srk'
predict(object, newdata, ...)
```

Arguments

`object`	An object of class `"srk"` returned by `srk`.
`newdata`	A data frame containing covariate and coordinate columns at prediction locations. Column names must match those used in the original `srk` call.
`...`	Additional arguments (currently unused).

Details

The prediction process follows three steps:

1. Singularity features are computed at prediction locations using combined training and prediction covariate data for neighbourhood completeness.
2. The random forest trend model is evaluated at prediction locations using the augmented feature set.
3. Residuals from training locations are interpolated to prediction locations via ordinary kriging, providing both predictions and uncertainty estimates.

Value

A data frame with columns:

x First coordinate of prediction location.

y Second coordinate of prediction location.

prediction Final SRK prediction (trend plus kriged residual).

trend Random forest trend estimate.

kriged_residual Ordinary kriging interpolation of residuals.

kriging_se Kriging standard error (prediction uncertainty).

References

Ren, K., Song, Y., Chen, M., and Yu, Q. (2026). A singularity regression kriging for spatial prediction. *GIScience & Remote Sensing*, **63**(1), 2690341. doi:10.1080/15481603.2026.2690341

Examples

```
set.seed(42)
train <- sim_srk_data(n_side = 10, scenario = "normal", seed = 42)
model <- srk(z ~ cov1, data = train, coords = ~x + y,
             scales = c(1, 2, 3, 4, 5), ntree = 100)

# Create prediction locations
pred_locs <- expand.grid(x = seq(2, 9, by = 1), y = seq(2, 9, by = 1))
pred_locs$cov1 <- rnorm(nrow(pred_locs), mean = mean(train$cov1))
preds <- predict(model, newdata = pred_locs)
head(preds)
```

`print.srk` *Print an SRK Model Object*

Description

Print an SRK Model Object

Usage

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

Arguments

`x`	An object of class "`srk`".
`...`	Additional arguments (currently unused).

Value

Invisibly returns `x`.

Examples

```
sim_data <- sim_srk_data(n_side = 10, scenario = "normal", seed = 42)
model <- srk(z ~ cov1, data = sim_data, coords = ~x + y,
             scales = c(1, 2, 3, 4, 5), ntree = 100)
print(model)
```

print.srk_cv *Print Cross-Validation Results*

Description

Print Cross-Validation Results

Usage

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

Arguments

`x`	An object of class `"srk_cv"`.
`...`	Additional arguments (currently unused).

Value

Invisibly returns `x`.

print.srk_sensitivity *Print Sensitivity Analysis Results*

Description

Print Sensitivity Analysis Results

Usage

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

Arguments

`x`	An object of class `"srk_sensitivity"`.
`...`	Additional arguments (currently unused).

Value

Invisibly returns `x`.

print.summary.srk — *Print Summary of an SRK Model*

Description

Print Summary of an SRK Model

Usage

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

Arguments

`x`	An object of class "`summary.srk`".
`...`	Additional arguments (currently unused).

Value

Invisibly returns `x`.

sim_srk_data — *Simulate Spatial Data for SRK Examples*

Description

Generates simulated spatial datasets on a regular grid with spatially autocorrelated fields and an associated covariate, following the simulation design described in Ren et al. (2026, Section 2.3).

Usage

```
sim_srk_data(
  n_side = 20L,
  scenario = c("normal", "skewed", "longtail"),
  seed = 42L
)
```

Arguments

`n_side`	Integer. Number of grid points per side. Total sample size is `n_side^2`. Default is 20.
`scenario`	Character. Distribution scenario for the response variable. One of "`normal`", "`skewed`", or "`longtail`". Default is "`normal`".
`seed`	Integer. Random seed for reproducibility. Default is 42.

Details

The data generation process follows the simulation design in Section 2.3.1 of Ren et al. (2026):

1. A spatially autocorrelated base field is generated using a spherical covariance model on a regular grid.
2. A covariate field is constructed to maintain a strong but imperfect spatial association with the base field.
3. The response variable is derived from the base field under one of three distributional scenarios: `"normal"` (linear shift), `"skewed"` (exponential transformation), or `"longtail"` (stronger exponential transformation).

Value

A data frame with columns:

x Horizontal grid coordinate.

y Vertical grid coordinate.

z Response variable.

cov1 Spatially autocorrelated covariate.

References

Ren, K., Song, Y., Chen, M., and Yu, Q. (2026). A singularity regression kriging for spatial prediction. *GIScience & Remote Sensing*, **63**(1), 2690341. doi:10.1080/15481603.2026.2690341

Examples

```
# Normal distribution scenario
sim_normal <- sim_srk_data(n_side = 10, scenario = "normal", seed = 42)
head(sim_normal)

# Skewed distribution scenario
sim_skew <- sim_srk_data(n_side = 10, scenario = "skewed", seed = 42)
summary(sim_skew$z)
```

`srk` *Fit a Singularity Regression Kriging Model*

Description

Fits the Singularity Regression Kriging (SRK) model for spatial prediction. SRK integrates covariate singularity feature construction, nonlinear trend estimation via random forest, and geostatistical interpolation of residuals using ordinary kriging.

Usage

```
srk(
  formula,
  data,
  coords,
  pred_data = NULL,
  scales = NULL,
  ntree = 500L,
  sd_threshold = 0.5,
  min_neighbours = 3L,
  min_scales = 2L,
  variogram_model = "auto"
)
```

Arguments

`formula`	A formula specifying the response variable and covariates, e.g., `z ~ cov1 + cov2`. The response variable must be numeric.
`data`	A data frame containing the response, covariates, and coordinate columns referenced in `formula` and `coords`.
`coords`	A one-sided formula specifying the coordinate columns in `data`, e.g., `~x + y`. Must reference exactly two columns.
`pred_data`	An optional data frame containing covariate and coordinate columns at prediction locations. Column names must match those in `data`. If provided, predictions are computed at these locations.
`scales`	A numeric vector of spatial scales for singularity computation. If `NULL`, defaults are chosen based on the coordinate range. See `compute_singularity` for details.
`ntree`	Integer. Number of trees in the random forest. Default is 500.
`sd_threshold`	Numeric. Minimum standard deviation for a singularity feature to be retained. Features with lower standard deviation are excluded. Default is 0.5.
`min_neighbours`	Integer. Minimum neighbours for singularity computation. Default is 3. See `compute_singularity`.
`min_scales`	Integer. Minimum scales for singularity computation. Default is 2. See `compute_singularity`.
`variogram_model`	Character. Variogram model type for residual kriging. Options are `"auto"` (automatic selection among Spherical, Exponential, and Gaussian models), `"Sph"`, `"Exp"`, or `"Gau"`. Default is `"auto"`.

Details

The SRK model follows three main steps as described in Ren et al. (2026):

1. **Singularity feature construction**: For each covariate, singularity indices are computed at multiple spatial scales using `compute_singularity`. Features with standard deviation below `sd_threshold` are discarded.

2. **Trend estimation**: A random forest (Breiman, 2001) is trained on the augmented feature set (original covariates plus retained singularity features) to estimate the spatial trend.
3. **Residual kriging**: The residuals from the random forest trend are interpolated using ordinary kriging with an automatically fitted variogram model to generate final predictions with uncertainty quantification.

Value

An object of class `"srk"` containing:

call The matched function call.

formula The model formula.

coord_names Names of coordinate columns.

cov_names Names of covariate columns.

train_coords Matrix of training coordinates.

train_covariates Data frame of training covariates.

observed Numeric vector of observed response values.

fitted_values Numeric vector of fitted values at training locations.

trend_fitted Numeric vector of random forest trend estimates at training locations.

residuals Numeric vector of residuals (observed minus trend).

trend_model The fitted `randomForest` object.

variogram_empirical The empirical variogram of residuals.

variogram_model The fitted variogram model.

singularity_indices A data frame of singularity indices at training locations.

retained_features Character vector of retained singularity feature names.

feature_importance Named numeric vector of variable importance scores from the random forest.

scales The spatial scales used.

sd_threshold The standard deviation threshold used.

n Number of training observations.

metrics A named list with training metrics: `R2`, `RMSE`, and `MAE`.

predictions If `pred_data` was provided, a data frame with columns `x`, `y`, `prediction`, `trend`, `kriged_residual`, and `kriging_se`.

References

Ren, K., Song, Y., Chen, M., and Yu, Q. (2026). A singularity regression kriging for spatial prediction. *GIScience & Remote Sensing*, **63**(1), 2690341. doi:10.1080/15481603.2026.2690341

Breiman, L. (2001). Random forests. *Machine Learning*, **45**(1), 5–32. doi:10.1023/A:1010933404324

Hengl, T., Heuvelink, G. B., and Rossiter, D. G. (2007). About regression-kriging: from equations to case studies. *Computers & Geosciences*, **33**(10), 1301–1315. doi:10.1016/j.cageo.2007.05.001

Examples

```
# Generate simulated data
sim_data <- sim_srk_data(n_side = 10, scenario = "normal", seed = 42)

# Fit SRK model
model <- srk(z ~ cov1, data = sim_data, coords = ~x + y,
             scales = c(1, 2, 3, 4, 5), ntree = 100)
print(model)
summary(model)
```

---

srk_block_cv *Spatial Block Cross-Validation for SRK Models*

Description

Performs spatial block cross-validation to evaluate the predictive accuracy of the SRK model. The study area is divided into spatial blocks, which are then assigned to folds for cross-validation, following the evaluation framework described in Ren et al. (2026, Section 3.2.3).

Usage

```
srk_block_cv(
  formula,
  data,
  coords,
  nfold = 5L,
  block_size,
  scales = NULL,
  ntree = 500L,
  sd_threshold = 0.5,
  min_neighbours = 3L,
  min_scales = 2L,
  variogram_model = "auto"
)
```

Arguments

formula	A formula specifying the response and covariates.
data	A data frame containing the variables.
coords	A one-sided formula specifying coordinate columns.
nfold	Integer. Number of cross-validation folds. Default is 5.
block_size	Numeric. Size of spatial blocks (in coordinate units).
scales	Numeric vector of spatial scales for singularity computation. See srk.
ntree	Integer. Number of trees in the random forest. Default is 500.

`sd_threshold`	Numeric. Singularity feature standard deviation threshold. Default is 0.5.
`min_neighbours`	Integer. Minimum neighbours for singularity computation. Default is 3.
`min_scales`	Integer. Minimum scales for singularity computation. Default is 2.
`variogram_model`	Character. Variogram model type. Default `"auto"`.

Details

The study area is divided into non-overlapping rectangular spatial blocks of the specified size. Each block is assigned to one of `nfold` folds. For each fold, the SRK model is fitted on all observations outside the fold, and predictions are generated for observations within the fold. Performance metrics (R-squared, RMSE, MAE) are computed per fold and overall.

Value

An object of class `"srk_cv"` containing:

observed Numeric vector of observed values.

predicted Numeric vector of cross-validated predictions.

fold_id Integer vector of fold assignments.

fold_metrics A data frame with per-fold R2, RMSE, and MAE.

overall_metrics A named list with overall R2, RMSE, and MAE.

nfold Number of folds used.

block_size Block size used.

References

Ren, K., Song, Y., Chen, M., and Yu, Q. (2026). A singularity regression kriging for spatial prediction. *GIScience & Remote Sensing*, **63**(1), 2690341. doi:10.1080/15481603.2026.2690341

Examples

```
set.seed(42)
sim_data <- sim_srk_data(n_side = 15, scenario = "normal", seed = 42)
cv_result <- srk_block_cv(z ~ cov1, data = sim_data, coords = ~x + y,
                          nfold = 3, block_size = 5,
                          scales = c(1, 2, 3, 4, 5), ntree = 100)
print(cv_result)
```

srk_sensitivity — *Parameter Sensitivity Analysis for SRK Models*

Description

Evaluates the robustness of the SRK model under different combinations of maximum singularity scale and singularity feature selection threshold, following the sensitivity analysis framework described in Ren et al. (2026, Section 4.4).

Usage

```
srk_sensitivity(
  formula,
  data,
  coords,
  scale_range,
  threshold_range,
  nfold = 5L,
  block_size,
  ntree = 500L,
  min_neighbours = 3L,
  min_scales = 2L,
  variogram_model = "auto",
  scale_step = 1
)
```

Arguments

`formula`	A formula specifying the response and covariates.
`data`	A data frame containing the variables.
`coords`	A one-sided formula specifying coordinate columns.
`scale_range`	Numeric vector of maximum singularity scales to test. For each value, a scale sequence from `scale_step` to that maximum is generated.
`threshold_range`	Numeric vector of standard deviation thresholds to test for singularity feature selection.
`nfold`	Integer. Number of cross-validation folds. Default is 5.
`block_size`	Numeric. Size of spatial blocks for cross-validation.
`ntree`	Integer. Number of trees in the random forest. Default is 500.
`min_neighbours`	Integer. Minimum neighbours for singularity computation. Default is 3.
`min_scales`	Integer. Minimum scales for singularity computation. Default is 2.
`variogram_model`	Character. Variogram model type. Default `"auto"`.
`scale_step`	Numeric. Step size for generating scale sequences. Default is 1.

Details

For each combination of maximum singularity scale and feature selection threshold, the function performs spatial block cross-validation using `srk_block_cv` and records the resulting performance metrics. This allows assessment of model robustness to parameter choices as described in the paper.

Value

An object of class `"srk_sensitivity"` containing:

results A data frame with columns `max_scale`, `threshold`, `R2`, `RMSE`, and `MAE` for each parameter combination.

scale_range The scale range tested.

threshold_range The threshold range tested.

References

Ren, K., Song, Y., Chen, M., and Yu, Q. (2026). A singularity regression kriging for spatial prediction. *GIScience & Remote Sensing*, **63**(1), 2690341. doi:10.1080/15481603.2026.2690341

Examples

```
set.seed(42)
sim_data <- sim_srk_data(n_side = 10, scenario = "normal", seed = 42)
sens <- srk_sensitivity(z ~ cov1, data = sim_data, coords = ~x + y,
                         scale_range = c(3, 5),
                         threshold_range = c(0.3, 0.5),
                         nfold = 3, block_size = 3, ntree = 50)
print(sens)
```

`srk_sim` *Simulated Spatial Data for SRK Examples*

Description

A simulated spatial dataset on a 20 by 20 regular grid with a spatially autocorrelated response variable and covariate, generated following the simulation design described in Ren et al. (2026, Section 2.3.1).

Usage

```
srk_sim
```

Format

A data frame with 400 rows and 4 variables:

x Horizontal grid coordinate (integer, 1 to 20).

y Vertical grid coordinate (integer, 1 to 20).

z Response variable (spatially autocorrelated, normal scenario).

cov1 Spatially autocorrelated covariate.

Source

Generated using `sim_srk_data` with `n_side = 20`, `scenario = "normal"`, and `seed = 42`.

References

Ren, K., Song, Y., Chen, M., and Yu, Q. (2026). A singularity regression kriging for spatial prediction. *GIScience & Remote Sensing*, **63**(1), 2690341. doi:10.1080/15481603.2026.2690341

Examples

```
data(srk_sim)
head(srk_sim)
summary(srk_sim)
```

`summary.srk` *Summary of an SRK Model*

Description

Provides a detailed summary of a fitted SRK model including variable importance, variogram parameters, and accuracy metrics.

Usage

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

Arguments

`object`	An object of class `"srk"`.
`...`	Additional arguments (currently unused).

Value

An object of class `"summary.srk"`.

Examples

```
sim_data <- sim_srk_data(n_side = 10, scenario = "normal", seed = 42)
model <- srk(z ~ cov1, data = sim_data, coords = ~x + y,
             scales = c(1, 2, 3, 4, 5), ntree = 100)
summary(model)
```

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