

# Package ‘georob’

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**Title** Robust Geostatistical Analysis of Spatial Data

**Description** Provides functions for efficiently fitting linear models with spatially correlated errors by robust (Kuensch et al. (2011) <[doi:10.3929/ethz-a-009900710](https://doi.org/10.3929/ethz-a-009900710)>) and Gaussian (Harville (1977) <[doi:10.1080/01621459.1977.10480998](https://doi.org/10.1080/01621459.1977.10480998)>) (Restricted) Maximum Likelihood and for computing robust and customary point and block external-drift Kriging predictions (Cressie (1993) <[doi:10.1002/9781119115151](https://doi.org/10.1002/9781119115151)>), along with utility functions for variogram modelling in ad hoc geostatistical analyses, model building, model evaluation by cross-validation, (conditional) simulation of Gaussian processes (Davies and Bryant (2013) <[doi:10.18637/jss.v055.i09](https://doi.org/10.18637/jss.v055.i09)>), unbiased back-transformation of Kriging predictions of log-transformed data (Cressie (2006) <[doi:10.1007/s11004-005-9022-8](https://doi.org/10.1007/s11004-005-9022-8)>).

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georob-package

*The georob Package*

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## Description

This is a summary of the features and functionality of **georob**, a package in R for customary and robust geostatistical analyses.

## Details

**georob** is a package for customary and robust analyses of geostatistical data. Such data, say  $y_i = y(\mathbf{s}_i)$ , are recorded at a set of locations,  $\mathbf{s}_i$ ,  $i = 1, 2, \dots, n$ , in a domain  $G \in \mathbb{R}^d$ ,  $d \in (1, 2, 3)$ , along with covariate information  $x_j(\mathbf{s}_i)$ ,  $j = 1, 2, \dots, p$ .

**Model:** We use the following model for the data  $y_i = y(\mathbf{s}_i)$ :

$$Y(\mathbf{s}_i) = Z(\mathbf{s}_i) + \varepsilon = \mathbf{x}(\mathbf{s}_i)^T \boldsymbol{\beta} + B(\mathbf{s}_i) + \varepsilon_i,$$

where  $Z(\mathbf{s}_i) = \mathbf{x}(\mathbf{s}_i)^T \boldsymbol{\beta} + B(\mathbf{s}_i)$  is the so-called signal,  $\mathbf{x}(\mathbf{s}_i)^T \boldsymbol{\beta}$  is the external drift,  $\{B(\mathbf{s})\}$  is an unobserved stationary or intrinsic spatial Gaussian random field with zero mean, and  $\varepsilon_i$  is an *i.i.d* error from a possibly long-tailed distribution with scale parameter  $\tau$  ( $\tau^2$  is usually called nugget effect). In vector form the model is written as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{B} + \boldsymbol{\varepsilon},$$

where  $\mathbf{X}$  is the model matrix with the rows  $\mathbf{x}(s_i)^\top$ .

The (generalized) covariance matrix of the vector of spatial Gaussian random effects  $\mathbf{B}$  is denoted by

$$E[\mathbf{B}\mathbf{B}^\top] = \mathbf{\Gamma}_\theta = \sigma_n^2 \mathbf{I} + \sigma^2 \mathbf{V}_\alpha = \sigma_B^2 \mathbf{V}_{\alpha,\xi} = \sigma_B^2 ((1-\xi) \mathbf{I} + \xi \mathbf{V}_\alpha),$$

where  $\sigma_n^2$  is the variance of seemingly uncorrelated micro-scale variation in  $B(s)$  that cannot be resolved with the chosen sampling design,  $\mathbf{I}$  is the identity matrix,  $\sigma^2$  is the variance of the captured auto-correlated variation in  $B(s)$ ,  $\sigma_B^2 = \sigma_n^2 + \sigma^2$  is the signal variance, and  $\xi = \sigma^2/\sigma_B^2$ . To estimate both  $\sigma_n^2$  and  $\tau^2$  (and not only their sum), one needs replicated measurements for some of the  $s_i$ .

We define  $\mathbf{V}_\alpha$  to be the (generalized) correlation matrix with elements

$$(\mathbf{V}_\alpha)_{ij} = \gamma_0 - \gamma(|\mathbf{A}(s_i - s_j)|),$$

where the constant  $\gamma_0$  is chosen large enough so that  $\mathbf{V}_\alpha$  is positive definite,  $\gamma(\cdot)$  is a valid stationary or intrinsic variogram, and  $\mathbf{A} = \mathbf{A}(\alpha, f_1, f_2; \omega, \phi, \zeta)$  is a matrix that is used to model geometrically anisotropic auto-correlation. In more detail,  $\mathbf{A}$  maps an arbitrary point on an ellipsoidal surface with constant semi-variance in  $\mathbb{R}^3$ , centred on the origin, and having lengths of semi-principal axes,  $\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3$ , equal to  $|\mathbf{p}_1| = \alpha$ ,  $|\mathbf{p}_2| = f_1 \alpha$  and  $|\mathbf{p}_3| = f_2 \alpha$ ,  $0 < f_2 \leq f_1 \leq 1$ , respectively, onto the surface of the unit ball centred on the origin.

The orientation of the ellipsoid is defined by the three angles  $\omega, \phi$  and  $\zeta$ :

$\omega$  is the azimuth of  $\mathbf{p}_1$  (= angle between north and the projection of  $\mathbf{p}_1$  onto the  $x$ - $y$ -plane, measured from north to south positive clockwise in degrees),

$\phi$  is 90 degrees minus the latitude of  $\mathbf{p}_1$  (= angle between the zenith and  $\mathbf{p}_1$ , measured from zenith to nadir positive clockwise in degrees), and

$\zeta$  is the angle between  $\mathbf{p}_2$  and the direction of the line, say  $y'$ , defined by the intersection between the  $x$ - $y$ -plane and the plane orthogonal to  $\mathbf{p}_1$  running through the origin ( $\zeta$  is measured from  $y'$  positive counter-clockwise in degrees).

The transformation matrix is given by

$$\mathbf{A} = \begin{pmatrix} 1/\alpha & 0 & 0 \\ 0 & 1/(f_1 \alpha) & 0 \\ 0 & 0 & 1/(f_2 \alpha) \end{pmatrix} (\mathbf{C}_1, \mathbf{C}_2, \mathbf{C}_3),$$

where

$$\mathbf{C}_1^\top = (\sin \omega \sin \phi, -\cos \omega \cos \zeta - \sin \omega \cos \phi \sin \zeta, \cos \omega \sin \zeta - \sin \omega \cos \phi \cos \zeta)$$

$$\mathbf{C}_2^\top = (\cos \omega \sin \phi, \sin \omega \cos \zeta - \cos \omega \cos \phi \sin \zeta, -\sin \omega \sin \zeta - \cos \omega \cos \phi \cos \zeta)$$

$$\mathbf{C}_3^\top = (\cos \phi, \sin \phi \sin \zeta, \sin \phi \cos \zeta)$$

To model geometrically anisotropic variograms in  $\mathbb{R}^2$  one has to set  $\phi = 90$  and  $f_2 = 1$ , and for  $f_1 = f_2 = 1$  one obtains the model for isotropic auto-correlation with range parameter  $\alpha$ . Note that for isotropic auto-correlation the software processes data for which  $d$  may exceed 3.

Two remarks are in order:

1. Clearly, the (generalized) covariance matrix of the observations  $\mathbf{Y}$  is given by

$$\text{Cov}[\mathbf{Y}, \mathbf{Y}^\top] = \tau^2 \mathbf{I} + \mathbf{\Gamma}_\theta.$$

2. Depending on the context, the term “variogram parameters” denotes sometimes all parameters of a geometrically anisotropic variogram model, but in places only the parameters of an isotropic variogram model, i.e.  $\sigma^2, \dots, \alpha, \dots$  and  $f_1, \dots, \zeta$  are denoted by the term “anisotropy parameters”. In the sequel  $\theta$  is used to denote all variogram and anisotropy parameters except the nugget effect  $\tau^2$ .

**Estimation:** The unobserved spatial random effects  $\mathbf{B}$  at the data locations  $\mathbf{s}_i$  and the model parameters  $\beta$ ,  $\tau^2$  and  $\theta^T = (\sigma^2, \sigma_n^2, \alpha, \dots, f_1, f_2, \omega, \phi, \zeta)$  are unknown and are estimated in **georob** either by Gaussian (Harville, 1977) or robust (Künsch et al., 2011) restricted maximum likelihood (REML) or Gaussian maximum likelihood (ML). Here  $\dots$  denote further parameters of the variogram such as the smoothness parameter of the Whittle-Matérn model.

In brief, the robust REML method is based on the insight that for given  $\theta$  and  $\tau^2$  the Kriging predictions (= BLUP) of  $\mathbf{B}$  and the generalized least squares (GLS = ML) estimates of  $\beta$  can be obtained simultaneously by maximizing

$$-\sum_i \left( \frac{y_i - \mathbf{x}(\mathbf{s}_i)^T \beta - B(\mathbf{s}_i)}{\tau} \right)^2 - \mathbf{B}^T \mathbf{\Gamma}_\theta^{-1} \mathbf{B}$$

with respect to  $\mathbf{B}$  and  $\beta$ , e.g. Harville (1977). Hence, the BLUP of  $\mathbf{B}$ , ML estimates of  $\beta$ ,  $\theta$  and  $\tau^2$  are obtained by maximizing

$$-\log(\det(\tau^2 \mathbf{I} + \mathbf{\Gamma}_\theta)) - \sum_i \left( \frac{y_i - \mathbf{x}(\mathbf{s}_i)^T \beta - B(\mathbf{s}_i)}{\tau} \right)^2 - \mathbf{B}^T \mathbf{\Gamma}_\theta^{-1} \mathbf{B}$$

jointly with respect to  $\mathbf{B}$ ,  $\beta$ ,  $\theta$  and  $\tau^2$  or by solving the respective estimating equations.

The estimating equations can then be robustified by

- replacing the standardized errors, say  $\varepsilon_i/\tau = (y_i - \mathbf{x}(\mathbf{s}_i)^T \beta - B(\mathbf{s}_i))/\tau$ , by a bounded or re-descending  $\psi$ -function,  $\psi_c(\varepsilon_i/\tau)$ , of them (e.g. Maronna et al, 2006, chap. 2) and by
- introducing suitable bias correction terms for Fisher consistency at the Gaussian model,

see Künsch et al. (2011) for details. The robustified estimating equations are solved numerically by a combination of iterated re-weighted least squares (IRWLS) to estimate  $\mathbf{B}$  and  $\beta$  for given  $\theta$  and  $\tau^2$  and nonlinear root finding by the function `nleqslv` of the R package `nleqslv` to get  $\theta$  and  $\tau^2$ . The robustness of the procedure is controlled by the tuning parameter  $c$  of the  $\psi_c$ -function. For  $c \geq 1000$  the algorithm computes Gaussian (RE)ML estimates and customary plug-in Kriging predictions. Instead of solving the Gaussian (RE)ML estimating equations, our software then maximizes the Gaussian (restricted) log-likelihood using `nlminb` or `optim`.

**georob** uses variogram models that were provided formerly by the now archived R package **RandomFields** and are now implemented in the function `gencorr` of **georob**. Currently, estimation of the parameters of the following models is implemented:

"RMaskey", "RMBessel", "RMcauchy", "RMcircular", "RMcubic", "RMDagum",  
 "RMDampedcos", "RMDewijsian", "RMexp" (default), "RMfbm", "RMgauss",  
 "RMgencauchy", "RMgenfbm", "RMgengneiting", "RMgneiting", "RMLgd",  
 "RMmatern", "RMPenta", "RMqexp", "RMspheric", "RMstable", "RMwave",  
 "RMwhittle".

For most variogram parameters, closed-form expressions of  $\partial\gamma/\partial\theta_i$  and  $\partial\gamma/\partial\tau^2$  are used in the computations. However, for the parameter  $\nu$  of the models "RMBessel", "RMmatern" and "RMwhittle"  $\partial\gamma/\partial\nu$  is evaluated numerically by the function `numericDeriv`, and this results in an increase in computing time when  $\nu$  is estimated.

**Prediction:** Customary and robust plug-in external drift point Kriging predictions can be computed for a non-sampled location  $s_0$  from the covariates  $\mathbf{x}(s_0)$ , the estimated parameters  $\hat{\boldsymbol{\beta}}$ ,  $\hat{\boldsymbol{\theta}}$  and the predicted random effects  $\hat{\mathbf{B}}$  by

$$\hat{Y}(s_0) = \hat{Z}(s_0) = \mathbf{x}(s_0)^T \hat{\boldsymbol{\beta}} + \boldsymbol{\gamma}_{\hat{\boldsymbol{\theta}}}^T(s_0) \boldsymbol{\Gamma}_{\hat{\boldsymbol{\theta}}}^{-1} \hat{\mathbf{B}},$$

where  $\boldsymbol{\Gamma}_{\hat{\boldsymbol{\theta}}}$  is the estimated (generalized) covariance matrix of  $\mathbf{B}$  and  $\boldsymbol{\gamma}_{\hat{\boldsymbol{\theta}}}(s_0)$  is the vector with the estimated (generalized) covariances between  $\mathbf{B}$  and  $B(s_0)$ . Kriging variances can be computed as well, based on approximated covariances of  $\hat{\mathbf{B}}$  and  $\hat{\boldsymbol{\beta}}$  (see *Künsch et al., 2011*, and appendices of *Nussbaum et al., 2014*, for details).

The package **georob** provides in addition software for computing customary and robust external drift *block* Kriging predictions. The required integrals of the generalized covariance function are computed by functions of the R package **constrainedKriging**.

**Functionality:** For the time being, the functionality of **georob** is limited to geostatistical analyses of *single* response variables. No software is currently available for customary and robust multivariate geostatistical analyses. **georob** offers functions for:

1. Robustly fitting a spatial linear model to data that are possibly contaminated by independent errors from a long-tailed distribution by robust REML (see functions [georob](#) — which also fits such models efficiently by Gaussian (RE)ML — [profilelogLik](#) and [control.georob](#)).
2. Extracting estimated model components (see [residuals.georob](#), [rstandard.georob](#), [ranef.georob](#)).
3. Robustly estimating sample variograms and for fitting variogram model functions to them (see [sample.variogram](#) and [fit.variogram.model](#)).
4. Model building by forward and backward selection of covariates for the external drift (see [waldtest.georob](#), [step.georob](#), [add1.georob](#), [drop1.georob](#), [extractAIC.georob](#), [logLik.georob](#), [deviance.georob](#)). For a robust fit, the log-likelihood is not defined. The function then computes the (restricted) log-likelihood of an equivalent Gaussian model with heteroscedastic nugget (see [deviance.georob](#) for details).
5. Assessing the goodness-of-fit and predictive power of the model by  $K$ -fold cross-validation (see [cv.georob](#) and [validate.predictions](#)).
6. Computing customary and robust external drift point and block Kriging predictions (see [predict.georob](#), [control.predict.georob](#)).
7. Unbiased back-transformation of both point and block Kriging predictions of log-transformed data to the original scale of the measurements (see [lgnpp](#)).
8. Computing unconditional and conditional Gaussian simulations from a fitted spatial linear model (see [condsim](#)).

#### Author(s)

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#### References

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- Künsch, H. R., Papritz, A., Schwierz, C. and Stahel, W. A. (in preparation) Robust Geostatistics.

Künsch, H. R., Papritz, A., Schwierz, C. and Stahel, W. A. (2011) Robust estimation of the external drift and the variogram of spatial data. Proceedings of the ISI 58th World Statistics Congress of the International Statistical Institute. doi:10.3929/ethza009900710

Maronna, R. A., Martin, R. D. and Yohai, V. J. (2006) *Robust Statistics Theory and Methods*, Wiley, Hoboken, doi:10.1002/0470010940.

Nussbaum, M., Papritz, A., Baltensweiler, A. and Walther, L. (2014) Estimating soil organic carbon stocks of Swiss forest soils by robust external-drift kriging. *Geoscientific Model Development*, 7, 1197–1210. doi:10.5194/gmd711972014.

### See Also

[georob](#) for (robust) fitting of spatial linear models;  
[georobObject](#) for a description of the class georob;  
[profilelogLik](#) for computing profiles of Gaussian likelihoods;  
[plot.georob](#) for display of RE(ML) variogram estimates;  
[control.georob](#) for controlling the behaviour of georob;  
[georobModelBuilding](#) for stepwise building models of class georob;  
[cv.georob](#) for assessing the goodness of a fit by georob;  
[georobMethods](#) for further methods for the class georob;  
[predict.georob](#) for computing robust Kriging predictions;  
[lgnpp](#) for unbiased back-transformation of Kriging prediction of log-transformed data;  
[georobSimulation](#) for simulating realizations of a Gaussian process from model fitted by georob;  
and finally  
[sample.variogram](#) and [fit.variogram.model](#) for robust estimation and modelling of sample variograms.

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compress

*Compact Storage of Symmetric and Triangular Matrices*

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### Description

The utility function `compress` stores symmetric or triangular matrices compactly by retaining only the diagonal and either the lower or upper off-diagonal elements. The function `expand` restores such compressed matrices again to a square form.

### Usage

```
compress(m)
```

```
expand(object)
```

**Arguments**

<code>m</code>	either a single symmetric, lower or upper triangular matrix or a list of such matrices. The type of <code>m</code> (or of its component matrices) must be defined by the attribute <code>struc</code> with possible values "sym" (symmetric), "lt" (lower triangular) or "ut" (upper triangular).
<code>object</code>	a single compressed matrix or a list of such matrices generated by <code>compress</code> , see <i>Value</i> . The type of <code>object</code> (or of its components) must be defined by the attribute <code>struc</code> with possible values "sym" (symmetric), "lt" (lower triangular) or "ut" (upper triangular).

**Value**

If `m` is a single square matrix then `compress` generates a compressed matrix, which is a list with two components:

<code>diag</code>	a vector with the diagonal elements of <code>m</code> .
<code>tri</code>	a vector with off-diagonal elements.

If `m` is a list of square matrices then the result is also a list of compressed matrices.

`expand` creates a square matrix if `object` is a list with components `diag` and `tri` and a list of square matrices if `object` is a list of such lists. If `m` or `objects` are lists that contain other components than square or compressed matrices then these additional components are returned unchanged.

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**See Also**

[georob](#) for (robust) fitting of spatial linear models.

**Examples**

```
data(meuse)

r.logzn.rob <- georob(log(zinc) ~ sqrt(dist) + ffreq, data = meuse,
  locations = ~ x + y, variogram.model = "RMexp",
  param = c(variance = 0.15, nugget = 0.05, scale = 200),
  tuning.psi = 1)

cov2cor(expand(r.logzn.rob[["cov"]][["cov.betahat"]]))
```

---

control.georob	<i>Control Parameters for georob</i>
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---

## Description

This page documents parameters used to control [georob](#). It describes the arguments of the functions `control.georob`, `param.transf`, `fwd.transf`, `dfwd.transf`, `bwd.transf`, `control.rq`, `control.nleqslv`, `control.nlminb` and `control.optim`, which all serve to control the behaviour of [georob](#).

## Usage

```
control.georob(ml.method = c("REML", "ML"), reparam = TRUE,
  maximizer = c("nlminb", "optim"), initial.param = TRUE,
  initial.fixef = c("lmrob", "rq", "lm"), bhat = NULL,
  min.rweight = 0.25,
  param.tf = param.transf(), fwd.tf = fwd.transf(),
  deriv.fwd.tf = dfwd.transf(), bwd.tf = bwd.transf(),
  psi.func = c("logistic", "t.dist", "huber"),
  irwls.maxiter = 50,
  irwls.ftol = 1.e-5, force.gradient = FALSE,
  min.condnum = 1.e-12, zero.dist = sqrt(.Machine[["double.eps"]]),
  error.family.estimation = c("gaussian", "long.tailed"),
  error.family.cov.effects = c("gaussian", "long.tailed"),
  error.family.cov.residuals = c("gaussian", "long.tailed"),
  cov.bhat = TRUE, full.cov.bhat = FALSE, cov.betahat = TRUE,
  cov.delta.bhat = TRUE, full.cov.delta.bhat = TRUE,
  cov.delta.bhat.betahat = TRUE,
  cov.ehat = TRUE, full.cov.ehat = FALSE,
  cov.ehat.p.bhat = FALSE, full.cov.ehat.p.bhat = FALSE,
  hessian = TRUE,
  rq = control.rq(), lmrob = lmrob.control(),
  nleqslv = control.nleqslv(),
  optim = control.optim(), nlminb = control.nlminb(),
  pcmp = control.pcmp(),...)

param.transf(variance = "log", snugget = "log", nugget = "log", scale = "log",
  alpha = c(
    RMaskey = "log", RMdewijsian = "logit2", RMfbm = "logit2", RMgencauchy = "logit2",
    RMgenfbm = "logit2", RMIgd = "identity", RMqexp = "logit1", RMstable = "logit2"
  ),
  beta = c(RMdagum = "logit1", RMgencauchy = "log", RMIgd = "log"),
  delta = "logit1", gamma = c(RMcauchy = "log", RMdagum = "logit1"),
  kappa = "logit3", lambda = "log", mu = "log", nu = "log",
  f1 = "log", f2 = "log", omega = "identity", phi = "identity", zeta = "identity")

fwd.transf(...)
```



```

dfwd.transf(...)

bwd.transf(...)

control.rq(tau = 0.5, rq.method = c("br", "fnb", "pfn"),
  rq.alpha = 0.1, ci = FALSE, iid = TRUE,
  interp = TRUE, tcrit = TRUE, rq.beta = 0.99995, eps = 1e-06,
  Mm.factor = 0.8, max.bad.fixup = 3, ...)

control.nleqslv(method = c("Broyden", "Newton"),
  global = c("dblDOG", "pwlDOG", "qline", "gline", "none"),
  xscalm = c("fixed", "auto"), control = list(ftol = 1e-04), ...)

control.optim(method = c("BFGS", "Nelder-Mead", "CG",
  "L-BFGS-B", "SANN", "Brent"), lower = -Inf, upper = Inf,
  control = list(reltol = 1e-05), ...)

control.nlminb(control = list(rel.tol = 1.e-5), lower = -Inf,
  upper = Inf, ...)

```

## Arguments

ml.method	a character keyword defining whether Gaussian maximum likelihood (ML) or restricted maximum likelihood (REML default) estimates will be computed (ignored if <code>tuning.psi &lt;= tuning.psi.nr</code> ).
reparam	a logical scalar. If TRUE (default) the re-parametrized variance parameters $\sigma_B^2$ , $\eta$ and $\xi$ are estimated by Gaussian (RE)ML, otherwise the original parameters $\tau^2$ , $\sigma_n^2$ and $\sigma^2$ (cf. subsection <i>Estimating variance parameters by Gaussian (RE)ML</i> , section <i>Details</i> of <code>georob</code> ).
maximizer	a character keyword defining whether the Gaussian (restricted) log-likelihood is maximized by <code>nlminb</code> (default) or <code>optim</code> .
initial.param	a logical scalar, controlling whether initial values of variogram parameters are computed for solving the robustified estimating equations of the variogram and anisotropy parameters. If <code>initial.param = TRUE</code> (default) robust initial values of parameters are computed by discarding outlying observations based on the “robustness weights” of the initial fit of the regression model by <code>lmrob</code> and fitting the spatial linear model by Gaussian REML to the pruned data set. For <code>initial.param = FALSE</code> no initial parameter values are computed and the estimating equations are solved with the initial values passed by <code>param</code> and <code>aniso</code> to <code>georob</code> (see <i>Details</i> of <code>georob</code> ).
initial.fixef	a character keyword defining whether the function <code>lmrob</code> or <code>rq</code> is used to compute robust initial estimates of the regression parameters $\beta$ (default “ <code>lmrob</code> ”). If the fixed effects model matrix has not full columns rank, then <code>lm</code> is used to compute initial values of the regression coefficients.
bhat	a numeric vector with initial values for the spatial random effects $\hat{B}$ , with $\hat{B} = \mathbf{0}$ if <code>bhat</code> is equal to NULL (default).

min.rweight	a positive numeric with the “robustness weight” of the initial <code>lmrob</code> fit that observations must exceed to be used for computing robust initial estimates of variogram parameters by setting <code>initial.param = TRUE</code> (see <code>georob</code> ; default 0.25).
param.tf	a function such as <code>param.transf</code> , which returns a named list of character strings that define the transformations to be applied to the variogram parameters for model fitting, see <i>Details</i> .
fwd.tf	a function such as <code>fwd.transf</code> , which returns a named list of invertible functions to be used to transform variogram parameters, see <i>Details</i> .
deriv.fwd.tf	a function such as <code>dfwd.transf</code> , which returns a named list of functions corresponding to the first derivatives of <code>fwd.tf</code> , see <i>Details</i> .
bwd.tf	a function such as <code>bwd.transf</code> , which returns the named list of inverse functions corresponding to <code>fwd.tf</code> , see <i>Details</i> .
psi.func	a character keyword defining what $\psi_c$ -function should be used for robust model fitting. Possible values are “logistic” (a scaled and shifted logistic CDF, default), “t.dist” (re-descending $\psi_c$ -function associated with Student $t$ -distribution with $c$ degrees of freedom) and “huber” (Huber’s $\psi_c$ -function).
irwls.maxiter	a positive integer equal to the maximum number of IRWLS iterations to solve the estimating equations of $\mathbf{B}$ and $\beta$ (default 50).
irwls.ftol	a positive numeric with the convergence criterion for IRWLS. Convergence is assumed if the objective function change of a IRWLS iteration does not exceed <code>ftol</code> .
force.gradient	a logical scalar controlling whether the estimating equations or the gradient of the Gaussian restricted log-likelihood are evaluated even if all variogram parameters are fixed (default FALSE).
min.condnum	a positive numeric with the minimum acceptable ratio of smallest to largest singular value of the model matrix $\mathbf{X}$ (default 1.e-12).
zero.dist	a positive numeric equal to the maximum distance, separating two sampling locations that are still considered as being coincident.
error.family.estimation	a character keyword, defining the probability distribution for $\varepsilon$ (default: “gaussian”) that is used to approximate the covariance of $\hat{\mathbf{B}}$ when solving the estimating equations, see <i>Details</i> .
error.family.cov.effects	a character keyword, defining the probability distribution for $\varepsilon$ (default: “gaussian”) that is used to approximate the covariances of $\hat{\beta}$ , $\hat{\mathbf{B}}$ and $\mathbf{B} - \hat{\mathbf{B}}$ , see <i>Details</i> .
error.family.cov.residuals	a character keyword, defining the probability distribution for $\varepsilon$ (default: “long.tailed”) that is used to approximate the covariances of $\hat{\varepsilon} = \mathbf{Y} - \mathbf{X}\hat{\beta} - \hat{\mathbf{B}}$ and $\hat{\varepsilon} + \hat{\mathbf{B}} = \mathbf{Y} - \mathbf{X}\hat{\beta}$ , see <i>Details</i> .
cov.bhat	a logical scalar controlling whether the covariances of $\hat{\mathbf{B}}$ are returned by <code>georob</code> (default FALSE).
full.cov.bhat	a logical scalar controlling whether the full covariance matrix (TRUE) or only the variance vector of $\hat{\mathbf{B}}$ is returned (default FALSE).

cov.betahat	a logical scalar controlling whether the covariance matrix of $\hat{\beta}$ is returned (default TRUE).
cov.delta.bhat	a logical scalar controlling whether the covariances of $B - \hat{B}$ are returned (default TRUE).
full.cov.delta.bhat	a logical scalar controlling whether the full covariance matrix (TRUE) or only the variance vector of $B - \hat{B}$ is returned (default TRUE).
cov.delta.bhat.betahat	a logical scalar controlling whether the covariance matrix of $B - \hat{B}$ and $\hat{\beta}$ is returned (default TRUE).
cov.ehat	a logical scalar controlling whether the covariances of $\hat{\varepsilon} = Y - X\hat{\beta} - \hat{B}$ are returned (default TRUE).
full.cov.ehat	a logical scalar controlling whether the full covariance matrix (TRUE) or only the variance vector of $\hat{\varepsilon} = Y - X\hat{\beta} - \hat{B}$ is returned (default FALSE).
cov.ehat.p.bhat	a logical scalar controlling whether the covariances of $\hat{\varepsilon} + \hat{B} = Y - X\hat{\beta}$ are returned (default FALSE).
full.cov.ehat.p.bhat	a logical scalar controlling whether the full covariance matrix (TRUE) or only the variance vector of $\hat{\varepsilon} + \hat{B} = Y - X\hat{\beta}$ is returned (default FALSE).
hessian	a logical scalar controlling whether for Gaussian (RE)ML the Hessian should be computed at the MLEs.
rq	a list of arguments passed to <code>rq</code> or a function such as <code>control.rq</code> that generates such a list (see <a href="#">rq</a> for allowed arguments).
lmrob	a list of arguments passed to the <code>control</code> argument of <code>lmrob</code> or a function such as <code>lmrob.control</code> that generates such a list (see <a href="#">lmrob.control</a> for allowed arguments).
nleqslv	a list of arguments passed to <code>nleqslv</code> or a function such as <code>control.nleqslv</code> that generates such a list (see <a href="#">nleqslv</a> for allowed arguments).
nlminb	a list of arguments passed to <code>nlminb</code> or a function such as <code>control.nlminb</code> that generates such a list (see <a href="#">nlminb</a> for allowed arguments).
optim	a list of arguments passed to <code>optim</code> or a function such as <code>control.optim</code> that generates such a list (see <a href="#">optim</a> for allowed arguments).
pcmp	a list of arguments, passed e.g. to <code>pmm</code> or a function such as <code>control.pcmp</code> that generates such a list (see <a href="#">control.pcmp</a> for allowed arguments).
...	for <code>fwd.transf</code> , <code>dfwd.transf</code> and <code>bwd.transf</code> a named vector of functions, extending the definition of transformations for variogram parameters (see <i>Details</i> ).
variance, nugget, nugget, scale, alpha, beta, delta, gamma, kappa, lambda, mu, nu	character strings with names of transformation functions of the variogram parameters.
f1, f2, omega, phi, zeta	character strings with names of transformation functions of the anisotropy variogram parameters.

tau, rq.method, rq.alpha, ci, iid, interp, tcrit  
 arguments passed as ... to `rq`. Note that only "br", "fnb" and "pfn" methods of `rq()` are currently supported.

rq.beta, eps, Mm.factor, max.bad.fixup  
 arguments passed as ... to `rq`.

method, global, xscalm, control, lower, upper, reltol, rel.tol  
 arguments passed to related arguments of `nleqslv`, `nlminb` and `optim`, respectively.

## Details

### Parameter transformations:

The arguments `param.tf`, `fwd.tf`, `deriv.fwd.tf`, `bwd.tf` define the transformations of the variogram parameters for RE(ML) estimation. Implemented are currently "log", "logit1", "logit2", "logit3" (various variants of logit-transformation, see code of function `fwd.transf`) and "identity" (= no) transformations. These are the possible values that the many arguments of the function `param.transf` accept (as quoted character strings) and these are the names of the list components returned by `fwd.transf`, `dfwd.transf` and `bwd.transf`. Additional transformations can be implemented by:

1. Extending the function definitions by arguments like  
`fwd.tf = fwd.transf(my.fun = function(x) your transformation),`  
`deriv.fwd.tf = dfwd.transf(my.fun = function(x) your derivative),`  
`bwd.tf = bwd.transf(my.fun = function(x) your back-transformation),`
2. Assigning to a given argument of `param.transf` the name of the new function, e.g.  
`variance = "my.fun".`

Note that the values given for the arguments of `param.transf` must match the names of the functions returned by `fwd.transf`, `dfwd.transf` and `bwd.transf`.

### Approximation of covariances of fixed and random effects and residuals:

The robustified estimating equations of robust REML depend on the covariances of  $\widehat{\mathbf{B}}$ . These covariances (and the covariances of  $\mathbf{B} - \widehat{\mathbf{B}}$ ,  $\widehat{\boldsymbol{\beta}}$ ,  $\widehat{\boldsymbol{\varepsilon}}$ ,  $\widehat{\boldsymbol{\varepsilon}} + \widehat{\mathbf{B}}$ ) are approximated by expressions that in turn depend on the variances of  $\boldsymbol{\varepsilon}$ ,  $\boldsymbol{\psi}(\boldsymbol{\varepsilon}/\tau)$  and the expectation of  $\boldsymbol{\psi}'(\boldsymbol{\varepsilon}/\tau)$  ( $= \partial/\partial\boldsymbol{\varepsilon} \boldsymbol{\psi}(\boldsymbol{\varepsilon}/\tau)$ ). The arguments `error.family.estimation`, `error.family.cov.effects` and `error.family.cov.residuals` control what parametric distribution for  $\boldsymbol{\varepsilon}$  is used to compute the variance of  $\boldsymbol{\varepsilon}$ ,  $\boldsymbol{\psi}(\boldsymbol{\varepsilon}/\tau)$  and the expectation of  $\boldsymbol{\psi}'(\boldsymbol{\varepsilon}/\tau)$  when

- solving the estimating equations (`error.family.estimation`),
- computing the covariances of  $\widehat{\boldsymbol{\beta}}$ ,  $\widehat{\mathbf{B}}$  and  $\mathbf{B} - \widehat{\mathbf{B}}$  (`error.family.cov.effects`) and
- computing the covariances of  $\widehat{\boldsymbol{\varepsilon}} = \mathbf{Y} - \mathbf{X}\widehat{\boldsymbol{\beta}} - \widehat{\mathbf{B}}$  and  $\widehat{\boldsymbol{\varepsilon}} + \widehat{\mathbf{B}} = \mathbf{Y} - \mathbf{X}\widehat{\boldsymbol{\beta}}$  (`error.family.cov.residuals`).

Possible options are: "gaussian" or "long.tailed". In the latter case the probability density function of  $\boldsymbol{\varepsilon}$  is assumed to be proportional to  $1/\tau \exp(-\rho_c(\boldsymbol{\varepsilon}/\tau))$ , where  $\rho_c(x) = \rho'_c(x)$ .

## Value

`control.georob`, `control.rq`, `control.nleqslv`, `control.optim` and `control.nlminb` all create lists with control parameters passed to `georob`, `rq`, `nleqslv`, `optim` or `nlminb`, see arguments

above and the help pages of the respective functions for information about the components of these lists. Note that the list returned by `control.georob` contains some components (`irwls.initial`, `tuning.psi.nr`, `cov.bhat.betahat`, `aux.cov.pred.target`) that cannot be changed by the user.

`param.transf` generates a list with character strings that define what transformations are used for estimating the variogram parameters, and `fwd.transf`, `bwd.transf` and `dfwd.transf` return lists of functions with forward and backward transformations and the first derivatives of the forward transformations, see section *Parameter transformations* above.

### Author(s)

Andreas Papritz <papritz@retired.ethz.ch>.

### See Also

[georobPackage](#) for a description of the model and a brief summary of the algorithms;

[georob](#) for (robust) fitting of spatial linear models;

[georobObject](#) for a description of the class `georob`;

[profilelogLik](#) for computing profiles of Gaussian likelihoods;

[plot.georob](#) for display of RE(ML) variogram estimates;

[georobModelBuilding](#) for stepwise building models of class `georob`;

[cv.georob](#) for assessing the goodness of a fit by `georob`;

[georobMethods](#) for further methods for the class `georob`;

[predict.georob](#) for computing robust Kriging predictions;

[lgpp](#) for unbiased back-transformation of Kriging prediction of log-transformed data;

[georobSimulation](#) for simulating realizations of a Gaussian process from model fitted by `georob`; and finally

[sample.variogram](#) and [fit.variogram.model](#) for robust estimation and modelling of sample variograms.

### Examples

```
data(meuse)

r.logzn.rob <- georob(log(zinc) ~ sqrt(dist), data = meuse, locations = ~ x + y,
  variogram.model = "RMexp",
  param = c(variance = 0.15, nugget = 0.05, scale = 200),
  tuning.psi = 1, control = control.georob(cov.bhat = TRUE,
  cov.ihat.p.bhat = TRUE, initial.fixef = "rq"), verbose = 2)

qqnorm(rstandard(r.logzn.rob, level = 0)); abline(0, 1)
qqnorm(ranef(r.logzn.rob, standard = TRUE)); abline(0, 1)
```

---

`cv`*Generic Cross-validation*

---

**Description**

Generic function for cross-validating models.

**Usage**

```
cv(object, ...)
```

**Arguments**

<code>object</code>	any model object.
<code>...</code>	additional arguments as required by the methods.

**Value**

will depend on the method function used; see the respective documentation.

**Author(s)**

Andreas Papritz <papritz@retired.ethz.ch>.

**See Also**

[georob](#) for (robust) fitting of spatial linear models;  
[cv.georob](#) for assessing the goodness of a model fitted by georob.

---

`cv.georob`*Cross-Validating a Spatial Linear Model Fitted by georob*

---

**Description**

This function assesses the goodness-of-fit of a spatial linear model by  $K$ -fold cross-validation. In more detail, the model is re-fitted  $K$  times by robust (or Gaussian) (RE)ML, excluding each time  $1/K$ th of the data. The re-fitted models are used to compute robust (or customary) external Kriging predictions for the omitted observations. If the response variable is log-transformed then the Kriging predictions can be optionally transformed back to the original scale of the measurements. S3methods for evaluating and plotting diagnostic summaries of the cross-validation errors are described for the function [validate.predictions](#).

**Usage**

```
## S3 method for class 'georob'
cv(object, formula = NULL, subset = NULL,
    method = c("block", "random"), nset = 10L, seed = NULL,
    sets = NULL, duplicates.in.same.set = TRUE, re.estimate = TRUE,
    param = object[["variogram.object"]][[1]][["param"]],
    fit.param = object[["variogram.object"]][[1]][["fit.param"]],
    aniso = object[["variogram.object"]][[1]][["aniso"]],
    fit.aniso = object[["variogram.object"]][[1]][["fit.aniso"]],
    variogram.object = NULL,
    use.fitted.param = TRUE, return.fit = FALSE,
    reduced.output = TRUE, lgn = FALSE,
    mfl.action = c("offset", "stop"),
    ncores = min(nset, parallel::detectCores()), verbose = 0, ...)
```

**Arguments**

object	an object of class of "georob", see <a href="#">georobObject</a> .
formula	an optional formula for the regression model passed by <a href="#">update</a> to <a href="#">georob</a> .
subset	an optional vector specifying a subset of observations to be used in the fitting process.
method	a character keyword, controlling whether subsets are formed by partitioning data set into contiguous spatial blocks by <a href="#">kmeans</a> (default) or randomly. Ignored if sets is non-NULL.
nset	a positive integer defining the number $K$ of subsets into which the data set is partitioned (default: $nset = 10$ ). Ignored if sets is non-NULL.
seed	an optional integer seed to initialize random number generation, see <a href="#">set.seed</a> . Ignored if sets is non-NULL.
sets	an optional vector of the same length as the response vector of the fitted model and with positive integers taking values in $(1, 2, \dots, K)$ , defining in this way the $K$ subsets into which the data set is split. If sets = NULL (default) the partition is randomly generated by <a href="#">kmeans</a> or <a href="#">runif</a> (using possibly seed).
duplicates.in.same.set	a logical scalar controlling whether replicated observations at a given location are assigned to the same subset when partitioning the data (default TRUE).
re.estimate	a logical scalar controlling whether the model is re-fitted to the reduced data sets before computing the Kriging predictions (TRUE, default) or whether the model passed in object is used to compute the predictions for the omitted observations, see <i>Details</i> .
param	a named numeric vector or a matrix or data frame with initial values of variogram parameters passed by <a href="#">update</a> to <a href="#">georob</a> . If param is a matrix (or a data frame) then it must have nset rows and <code>length(object[["variogram.object"]][[1]][["param"]])</code> columns with initial values of variogram parameters for the nset cross-validation sets, and <code>colnames(param)</code> must match <code>names(object[["variogram.object"]][[1]][["param"]])</code> .

<code>fit.param</code>	<p>a named logical vector or a matrix or data frame defining which variogram parameters should be adjusted by <code>update</code>. If <code>fit.param</code> is a matrix (or a data frame) then it must have <code>nset</code> rows and <code>length(object[["variogram.object"]][[1]][["fit.param"]])</code> columns with variogram parameter fitting flags for the <code>nset</code> cross-validation sets, and <code>colnames(param)</code> must match <code>names(object[["variogram.object"]][[1]][["fit.param"]])</code>.</p>
<code>aniso</code>	<p>a named numeric vector or a matrix or data frame with initial values of anisotropy parameters passed by <code>update</code> to <code>georob</code>. If <code>aniso</code> is a matrix (or a data frame) then it must have <code>nset</code> rows and <code>length(object[["variogram.object"]][[1]][["aniso"]])</code> columns with initial values of anisotropy parameters for the <code>nset</code> cross-validation sets, and <code>colnames(aniso)</code> must match <code>names(object[["variogram.object"]][[1]][["aniso"]])</code>.</p>
<code>fit.aniso</code>	<p>a named logical vector or a matrix or data frame defining which anisotropy parameters should be adjusted by <code>update</code>. If <code>fit.aniso</code> is a matrix (or a data frame) then it must have <code>nset</code> rows and <code>length(object[["variogram.object"]][[1]][["fit.aniso"]])</code> columns with anisotropy parameter fitting flags for the <code>nset</code> cross-validation sets, and <code>colnames(param)</code> must match <code>names(object[["variogram.object"]][[1]][["fit.aniso"]])</code>.</p>
<code>variogram.object</code>	<p>an optional list that gives initial values for fitting a possibly nested variogram model for the cross-validation sets. Each component is a list with the following components:</p> <ul style="list-style-type: none"> <li>• <code>param</code>: an optional named numeric vector or a matrix or data frame with initial values of variogram parameters passed by <code>update</code> to <code>georob</code>. If <code>param</code> is a matrix (or a data frame) then it must have <code>nset</code> rows and <code>length(object[["variogram.object"]][[i]][["param"]])</code> columns with initial values of variogram parameters for the <code>nset</code> cross-validation sets (<math>i</math> is the <math>i</math>th variogram structure), and <code>colnames(param)</code> must match <code>names(object[["variogram.object"]][[i]][["param"]])</code>.</li> <li>• <code>fit.param</code>: an optional named logical vector or a matrix or data frame defining which variogram parameters should be adjusted by <code>update</code>. If <code>fit.param</code> is a matrix (or a data frame) then it must have <code>nset</code> rows and <code>length(object[["variogram.object"]][[i]][["fit.param"]])</code> columns with variogram parameter fitting flags for the <code>nset</code> cross-validation sets (<math>i</math> is the <math>i</math>th variogram structure), and <code>colnames(param)</code> must match <code>names(object[["variogram.object"]][[i]][["fit.param"]])</code>.</li> <li>• <code>aniso</code>: an optional named numeric vector or a matrix or data frame with initial values of anisotropy parameters passed by <code>update</code> to <code>georob</code>. If <code>aniso</code> is a matrix (or a data frame) then it must have <code>nset</code> rows and <code>length(object[["variogram.object"]][[i]][["aniso"]])</code> columns with initial values of anisotropy parameters for the <code>nset</code> cross-validation sets (<math>i</math> is the <math>i</math>th variogram structure), and <code>colnames(aniso)</code> must match <code>names(object[["variogram.object"]][[i]][["aniso"]])</code>.</li> <li>• <code>fit.aniso</code>: an optional named logical vector or a matrix or data frame defining which anisotropy parameters should be adjusted by <code>update</code>. If</li> </ul>



`fit.aniso` is a matrix (or a data frame) then it must have `nset` rows and `length(object[["variogram.object"]][[i]][["fit.aniso"]])` columns with anisotropy parameter fitting flags for the `nset` cross-validation sets ( $i$  is the  $i$ th variogram structure), and `colnames(param)` must match `names(object[["variogram.object"]][[i]][["fit.aniso"]])`.

<code>use.fitted.param</code>	a logical scalar controlling whether fitted values of <code>param</code> (and <code>aniso</code> are used as initial values when variogram parameters are fitted for the cross-validation sets (default TRUE).
<code>return.fit</code>	a logical scalar controlling whether information about the fit should be returned when re-estimating the model with the reduced data sets (default FALSE).
<code>reduced.output</code>	a logical scalar controlling whether the complete fitted model objects, fitted to the reduced data sets, are returned (FALSE) or only some components (TRUE, default, see <i>Value</i> ). Ignored if <code>return.fit = FALSE</code> .
<code>lgn</code>	a logical scalar controlling whether Kriging predictions of a log-transformed response should be transformed back to the original scale of the measurements (default FALSE).
<code>mfl.action</code>	a character keyword controlling what is done when some levels of factor(s) are not present in any of the subsets used to fit the model. The function either stops ("stop") or treats the respective factors as model offset ("offset", default).
<code>ncores</code>	a positive integer controlling how many cores are used for parallelized computations, see <i>Details</i> .
<code>verbose</code>	a positive integer controlling logging of diagnostic messages to the console during model fitting. Passed by <code>update</code> to <code>georob</code> .
<code>...</code>	additional arguments passed by <code>update</code> to <code>georob</code> , see <i>Details</i> .

## Details

**Note** that *the data frame passed as data argument to georob must exist in the user workspace when calling cv.georob*.

`cv.georob` uses the packages **parallel** and **snowfall** for parallelized computations. By default, the function uses  $K$  CPUs but not more than are physically available (as returned by `detectCores`).

`cv.georob` uses the function `update` to re-estimated the model with the reduced data sets. Therefore, any argument accepted by `georob` except `data` can be changed when re-fitting the model. Some of them (e.g. `formula`, `subset`, etc.) are explicit arguments of `cv.georob`, but also the remaining ones can be passed by `...` to the function.

Practitioners in geostatistics commonly cross-validate a fitted model without re-estimating the model parameters with the reduced data sets. This is clearly an unsound practice (see *Hastie et al., 2009, sec. 7.10*). Therefore, the argument `re.estimate` should always be set to TRUE. The alternative is provided only for historic reasons.

## Value

The method `cv.georob` returns an object of class `cv.georob`, which is a list with the two components `pred` and `fit`.

pred is a data frame with the coordinates and the cross-validation prediction results with the following variables:

subset	an integer vector defining to which of the $K$ subsets an observation was assigned.
data	the values of the (possibly log-transformed) response.
pred	the Kriging predictions.
se	the Kriging standard errors.

If lgn = TRUE then pred has the additional variables:

lgn.data	the untransformed response.
lgn.pred	the unbiased back-transformed predictions of a log-transformed response.
lgn.se	the Kriging standard errors of the back-transformed predictions of a log-transformed response.

The second component fit contains either the full outputs of georob, fitted for the  $K$  reduced data sets (reduced.output = FALSE), or  $K$  lists with the components tuning.psi, converged, convergence.code, gradient, variogram.object, coefficients along with the standard errors of  $\hat{\beta}$ , see [georobObject](#).

#### Author(s)

Andreas Papritz <papritz@retired.ethz.ch>.

#### References

Hastie, T., Tibshirani, R. and Friedman, J. (2009) *The Elements of Statistical Learning; Data Mining, Inference and Prediction*, Springer, New York, doi:10.1007/9780387848587

#### See Also

[georobPackage](#) for a description of the model and a brief summary of the algorithms;  
[georob](#) for (robust) fitting of spatial linear models;  
[georobObject](#) for a description of the class georob;  
[profilelogLik](#) for computing profiles of Gaussian likelihoods;  
[plot.georob](#) for display of RE(ML) variogram estimates;  
[control.georob](#) for controlling the behaviour of georob;  
[georobModelBuilding](#) for stepwise building models of class georob;  
[georobMethods](#) for further methods for the class georob;  
[predict.georob](#) for computing robust Kriging predictions;  
[validate.predictions](#) for validating Kriging predictions;  
[lgnpp](#) for unbiased back-transformation of Kriging prediction of log-transformed data;  
[georobSimulation](#) for simulating realizations of a Gaussian process from model fitted by georob;  
 and finally  
[sample.variogram](#) and [fit.variogram.model](#) for robust estimation and modelling of sample variograms.

**Examples**

```
## define number of cores for parallel computations
if(interactive()) ncpu <- 10L else ncpu <- 1L

data(meuse)

r.logzn <- georob(log(zinc) ~ sqrt(dist), data = meuse, locations = ~ x + y,
  variogram.model = "RMexp",
  param = c(variance = 0.15, nugget = 0.05, scale = 200),
  tuning.psi = 1000)

if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s
  r.logzn.cv.1 <- cv(r.logzn, seed = 1, lgn = TRUE, ncores = 1, verbose = 1)

  r.logzn.cv.2 <- cv(r.logzn, formula = .~. + ffreq, seed = 1, lgn = TRUE,
    ncores = ncpu)

  plot(r.logzn.cv.1, type = "bs")
  plot(r.logzn.cv.2, type = "bs", add = TRUE, col = "red")

  legend("topright", lty = 1, col = c("black", "red"), bty = "n",
    legend = c("log(Zn) ~ sqrt(dist)", "log(Zn) ~ sqrt(dist) + ffreq"))
}
```

---

 default.aniso

*Setting Default Values of Variogram Parameters*


---

**Description**

Auxiliary functions to set sensible default values for anisotropy parameters and for controlling what variogram and anisotropy parameters should be estimated.

**Usage**

```
default.aniso(f1 = 1., f2 = 1., omega = 90., phi = 90., zeta = 0.)
```

```
default.fit.param(
  variance = TRUE, snugget = FALSE, nugget = TRUE, scale = TRUE,
  alpha = FALSE, beta = FALSE, delta = FALSE, gamma = FALSE,
  kappa = FALSE, lambda = FALSE, mu = FALSE, nu = FALSE)
```

```
default.fit.aniso(f1 = FALSE, f2 = FALSE, omega = FALSE,
  phi = FALSE, zeta = FALSE)
```

**Arguments**

variance      variance (sill  $\sigma^2$ ) of the auto-correlated component of the Gaussian random field  $B(\mathbf{s})$ .

snugget	variance (spatial nugget $\sigma_n^2$ ) of the seemingly spatially uncorrelated component of $B(\mathbf{s})$ (micro-scale spatial variation; default value snugget = 0).
nugget	variance (nugget $\tau^2$ ) of the independent error $\varepsilon(\mathbf{s})$ .
scale	range parameter ( $\alpha$ ) of the variogram.
alpha, beta, delta, gamma, kappa, lambda, mu, nu	names of additional variogram parameters such as the smoothness parameter $\nu$ of the Whittle-Matérn model (see <a href="#">gencorr</a> and <a href="#">param.names</a> ).
f1	positive ratio $f_1$ of lengths of second and first semi-principal axes of an ellipsoidal surface with constant semi-variance in $\mathbb{R}^3$ (default f1 = 1), see subsection <i>Model</i> of <a href="#">georobPackage</a> .
f2	positive ratio $f_2$ of lengths of third and first semi-principal axes of the semi-variance ellipsoid (default f2 = 1), see subsection <i>Model</i> of <a href="#">georobPackage</a> .
omega	azimuth in degrees of the first semi-principal axis of the semi-variance ellipsoid (default omega = 90), see subsection <i>Model</i> of <a href="#">georobPackage</a> .
phi	90 degrees minus altitude of the first semi-principal axis of the semi-variance ellipsoid (default phi = 90), see subsection <i>Model</i> of <a href="#">georobPackage</a> .
zeta	angle in degrees between the second semi-principal axis and the direction of the line defined by the intersection between the $x$ - $y$ -plane and the plane orthogonal to the first semi-principal axis of the semi-variance ellipsoid through the origin (default zeta = 0), see subsection <i>Model</i> of <a href="#">georobPackage</a> .

### Value

Either a named numeric vector with initial values of anisotropy parameters (default.aniso) or named logical vectors, controlling what parameters should be estimated (default.fit.param, default.fit.aniso).

### Author(s)

Andreas Papritz <papritz@retired.ethz.ch>.

### See Also

[georobPackage](#) for a description of the model and a brief summary of the algorithms;  
[georob](#) for (robust) fitting of spatial linear models.

### Examples

```
default.aniso(f1 = 0.5, omega = 45)
default.fit.param(scale=FALSE, alpha = TRUE)
default.fit.aniso(f1 = TRUE, omega = TRUE)
```

---

`elevation`*Elevation Data*

---

**Description**

Surface elevation data taken from *Davis (1972)*.

**Usage**

```
data(elevation)
```

**Format**

A data frame with 52 observations on the following 3 variables:

`x` a numeric vector with the easting coordinate in multiples of 50 feet.

`y` a numeric vector with the northing coordinate in multiples of 50 feet..

`height` a numeric vector with the elevation in multiples of 10 feet.

**Note**

The data were imported from the package **geoR**.

**Source**

Davis, J.C. (1973) *Statistics and Data Analysis in Geology*, Wiley, New York.

**Examples**

```
data(elevation)
summary(elevation)
```

---

`fit.variogram.model`*Fitting Model Functions to Sample Variograms*

---

**Description**

The function `fit.variogram.model` fits a variogram model to a sample variogram by (weighted) non-linear least squares. The function `control.fit.variogram.model` generates a list with steering parameters which control `fit.variogram.model`. There are `print`, `summary` and `lines` methods for summarizing and displaying fitted variogram models.

**Usage**

```

fit.variogram.model(sv,
  variogram.model = c("RMexp", "RMaskey", "RMBessel", "RMcauchy",
    "RMcircular", "RMcubic", "RMDagum", "RMDampedcos", "RMDewijsian",
    "RMfbm", "RMgauss", "RMgencauchy", "RMgenfbm", "RMgengneiting",
    "RMgneiting", "RMLgd", "RMmatern", "RMpenta", "RMqexp",
    "RMspheric", "RMstable", "RMwave", "RMwhittle"),
  param, fit.param = default.fit.param()[names(param)],
  aniso = default.aniso(), fit.aniso = default.fit.aniso(),
  variogram.object = NULL,
  max.lag = max(sv[["lag.dist"]]), min.npairs = 30,
  weighting.method = c("cressie", "equal", "npairs"),
  control = control.fit.variogram.model(),
  verbose = 0)

control.fit.variogram.model(maximizer = c("nlminb", "optim"),
  param.tf = param.transf(), fwd.tf = fwd.transf(),
  deriv.fwd.tf = dfwd.transf(), bwd.tf = bwd.transf(),
  hessian = TRUE, optim = control.optim(), nlminb = control.nlminb())

## S3 method for class 'fitted.variogram'
print(x, digits = max(3, getOption("digits") - 3), ...)

## S3 method for class 'fitted.variogram'
summary(object, correlation = FALSE, signif = 0.95, ...)

## S3 method for class 'fitted.variogram'
lines(x, what = c("variogram", "covariance", "correlation"),
  from = 1.e-6, to, n = 501, xy.angle = 90, xz.angle = 90,
  col = 1:length(xy.angle), pch = 1:length(xz.angle), lty = "solid", ...)

```

**Arguments**

**sv** an object of class `sample.variogram`, see [sample.variogram](#).

**variogram.model** a character keyword defining the variogram model to be fitted. Currently, most basic variogram models provided formerly by the now archived package **RandomFields** can be fitted (see *Details* of [georob](#) and [gencorr](#)).

**param** a named numeric vector with initial values of the variogram parameters. The following parameter names are allowed (see *Details* of [georob](#) and [georobPackage](#) for information about the parametrization of variogram models):

- **variance**: variance (sill  $\sigma^2$ ) of the auto-correlated component of the Gaussian random field  $B(s)$ .
- **snugget**: variance (spatial nugget  $\sigma_n^2$ ) of the seemingly spatially uncorrelated component of  $B(s)$  (micro-scale spatial variation; default value snugget = 0).

- nugget: variance (nugget  $\tau^2$ ) of the independent errors  $\varepsilon(\mathbf{s})$ .
  - scale: range parameter ( $\alpha$ ) of the variogram.
  - names of additional variogram parameters such as the smoothness parameter  $\nu$  of the Whittle-Matérn model (see [gencorr](#) and [param.names](#)).
- `fit.param` a named logical vector (or a function such as [default.fit.param](#) that creates this vector) with the same names as used for `param`, defining which parameters are adjusted (TRUE) and which are kept fixed at their initial values (FALSE) when fitting the model.
- `aniso` a named numeric vector with initial values (or a function such as [default.aniso](#) that creates this vector) for fitting geometrically anisotropic variogram models. The names of `aniso` are matched against the following names (see *Details* and [georobPackage](#) for information about the parametrization of variogram models):
- `f1`: ratio  $f_1$  of lengths of second and first semi-principal axes of an ellipsoidal surface with constant semi-variance in  $\mathbb{R}^3$  (default `f1 = 1`).
  - `f2`: ratio  $f_2$  of lengths of third and first semi-principal axes of the semi-variance ellipsoid (default `f2 = 1`).
  - `omega`: azimuth in degrees of the first semi-principal axis of the semi-variance ellipsoid (default `omega = 90`).
  - `phi`: 90 degrees minus altitude of the first semi-principal axis of the semi-variance ellipsoid (default `phi = 90`).
  - `zeta`: angle in degrees between the second semi-principal axis and the direction of the line defined by the intersection between the  $x$ - $y$ -plane and the plane orthogonal to the first semi-principal axis of the semi-variance ellipsoid through the origin (default `zeta = 0`).
- `fit.aniso` a named logical vector (or a function such as [default.fit.aniso](#) that creates this vector) with the same names as used for `aniso`, defining which parameters are adjusted (TRUE) and which are kept fixed at their initial values (FALSE) when fitting the model.
- `variogram.object` an optional list that defines a possibly nested variogram model. Each component is itself a list with the following components:
- `variogram.model`: a character keyword defining the variogram model, see respective argument above.
  - `param`: a named numeric vector with initial values of the variogram parameters, see respective argument above.
  - `fit.param`: a named logical vector defining which parameters are adjusted, see respective argument above.
  - `aniso`: a named numeric vector with initial values for fitting geometrically anisotropic variogram models, see respective argument above.
  - `fit.param`: a named logical vector defining which anisotropy parameters are adjusted, see respective argument above.

Note that the arguments `variogram.model`, `param`, `fit.param`, `aniso` and `fit.aniso` are ignored when `variogram.object` is passed to `fit.variogram.model`.

max.lag	a positive numeric defining the maximum lag distance to be used for fitting or plotting variogram models (default all lag classes).
min.npairs	a positive integer defining the minimum number of data pairs required so that a lag class is used for fitting a variogram model (default 30).
weighting.method	a character keyword defining the weights for non-linear least squares. Possible values are: <ul style="list-style-type: none"> <li>• "equal": no weighting ,</li> <li>• "npairs": weighting by number of data pairs in a lag class,</li> <li>• "cressie": "Cressie's weights" (default, see <i>Cressie, 1993, sec. 2.6.2</i>).</li> </ul>
verbose	a positive integer controlling logging of diagnostic messages to the console during model fitting.
control	a list with the components maximizer, param.tf, fwd.tf, bwd.tf, hessian, optim and nlminb or a function such as control.fit.variogram.model that generates such a list. See <a href="#">control.georob</a> for information on maximizer, param.tf, fwd.tf, bwd.tf, hessian, optim and nlminb.
maximizer	a character keyword defining the optimizer for nonlinear least squares. Possible values are <a href="#">nlminb</a> (default) or <a href="#">optim</a> .
hessian	a logical scalar controlling whether the Hessian should be computed at the non-linear least squares estimates.
param.tf	a function such as <a href="#">param.transf</a> , which returns a named vector of character strings that define the transformations to be applied to the variogram parameters for model fitting, see <a href="#">control.georob</a> .
fwd.tf	a function such as <a href="#">fwd.transf</a> , which returns a named list of invertible functions to be used to transform variogram parameters, see <a href="#">control.georob</a> .
deriv.fwd.tf	a function such as <a href="#">dfwd.transf</a> , which returns a named list of functions corresponding to the first derivatives of fwd.tf, see <a href="#">control.georob</a> .
bwd.tf	a function such as <a href="#">bwd.transf</a> , which returns the named list of inverse functions corresponding to fwd.tf, see <a href="#">control.georob</a> .
nlminb	a list of arguments passed to nlminb or a function such as <a href="#">control.nlminb</a> that generates such a list (see <a href="#">nlminb</a> for allowed arguments).
optim	a list of arguments passed to optim or a function such as <a href="#">control.optim</a> that generates such a list (see <a href="#">optim</a> for allowed arguments).
object, x	an object of class fitted.variogram.
digits	a positive integer indicating the number of decimal digits to print.
correlation	a logical scalar controlling whether the correlation matrix of the fitted variogram parameters is computed (default FALSE).
signif	a numeric with the confidence level for computing confidence intervals for variogram parameters (default 0.95).
what	a character keyword with the quantity that should be displayed (default "variogram").
from	a numeric with the minimal lag distance used in plotting variogram models.
to	a numeric with the maximum lag distance used in plotting variogram models (default: largest lag distance of current plot).



n	a positive integer specifying the number of equally spaced lag distances for which semi-variances are evaluated in plotting variogram models (default 501).
xy.angle	a numeric vector with azimuth angles (in degrees, clockwise positive from north) in $x$ - $y$ -plane for which semi-variances should be plotted.
xz.angle	a numeric vector with angles in $x$ - $z$ -plane (in degrees, clockwise positive from zenith to south) for which semi-variances should be plotted.
col	a vector with colours of curves to distinguish curves relating to different azimuth angles in $x$ - $y$ -plane.
pch	a vector with the plotting symbols added to lines to distinguish curves relating to different angles in $x$ - $z$ -plane.
lty	a vector with the line types for plotting variogram models.
...	additional arguments passed to methods.

### Details

The parametrization of geometrically anisotropic variograms is described in detail in [georobPackage](#), and the section *Details* of [georob](#) describes how the parameter estimates are constrained to permissible ranges. The same mechanisms are used in `fit.variogram.model`.

The method `summary` computes confidence intervals of the estimated variogram and anisotropy parameters from the Hessian matrix of the residual sums of squares, based on the asymptotic normal distribution of least squares estimates. Note that the Hessian matrix with respect to the *transformed* variogram and anisotropy parameters is used for this. Hence the inverse Hessian matrix is the covariance matrix of the transformed parameters, confidence intervals are first computed for the transformed parameters and the limits of these intervals are transformed back to the original scale of the parameters. Optionally, `summary` reports the correlation matrix of the *transformed* parameters, also computed from the Hessian matrix.

### Value

The function `fit.variogram.model` generates an object of class `fitted.variogram` which is a list with the following components:

sse	the value of the object function (weighted residual sum of squares) evaluated at the solution.
variogram.object	the estimated parameters of a possibly nested variograms model. This is a list that contains for each variogram model structure the following components: <ul style="list-style-type: none"> <li>• <code>variogram.model</code>: the name of the fitted parametric variogram model.</li> <li>• <code>param</code>: a named numeric vector with the (estimated) variogram parameters.</li> <li>• <code>fit.param</code>: a named logical vector with the flags defining what variogram parameters were estimated.</li> <li>• <code>isotropic</code>: logical indicating whether an isotropic variogram was fitted.</li> <li>• <code>aniso</code>: a named numeric vector with the (estimated) anisotropy parameters.</li> <li>• <code>fit.aniso</code>: a named logical vector with the flags defining what anisotropy parameters were estimated.</li> </ul>

	<ul style="list-style-type: none"> <li>• <code>sincos</code>: a list with <code>sin</code> and <code>cos</code> of the angles <math>\omega</math>, <math>\phi</math> and <math>\zeta</math> that define the orientation of the anisotropy ellipsoid.</li> <li>• <code>rotmat</code>: the matrix <math>(C_1, C_2, C_3)</math> (see <a href="#">georobPackage</a>).</li> <li>• <code>sclmat</code>: a vector with the elements <math>1, 1/f_1, 1/f_2</math> (see <a href="#">georobPackage</a>).</li> </ul>
<code>param.tf</code>	a character vector listing the transformations of the variogram parameters used for model fitting.
<code>fwd.tf</code>	a list of functions for variogram parameter transformations.
<code>bwd.tf</code>	a list of functions for <i>inverse</i> variogram parameter transformations.
<code>converged</code>	a logical scalar indicating whether numerical maximization by <code>nlminb</code> or <code>optim</code> converged.
<code>convergence.code</code>	a diagnostic integer issued by <code>nlminb</code> or <code>optim</code> (component convergence) about convergence.
<code>iter</code>	a named integer vector of length two with the number of function and gradient evaluations by <code>nlminb</code> or <code>optim</code> .
<code>call</code>	the matched call.
<code>residuals</code>	a numeric vector with the residuals, that is the sample semi-variance minus the fitted values.
<code>fitted</code>	a numeric vector with the modelled semi-variances.
<code>weights</code>	a numeric vector with the weights used for fitting.
<code>hessian.tfp</code>	a symmetric matrix with the Hessian at the solution with respect to the transformed variogram and anisotropy parameters (missing if <code>hessian</code> is false). This Hessian is used by <code>summary.fitted.variogram</code> to compute confidence intervals for the estimated parameters.
<code>hessian.ntfp</code>	a symmetric matrix with the Hessian at the solution with respect to the non-transformed variogram and anisotropy parameters (missing if <code>hessian</code> is false).

The function `control.fit.variogram.model` returns a list with parameters to steer `fit.variogram.model`, see arguments of the function above for its components.

The method `print.fitted.variogram` invisibly returns the fitted variogram model unchanged.

The method `summary.fitted.variogram` returns an object of class `summary.fitted.variogram` which is a list containing a subset of the components of the fitted variogram object (`call`, `residuals`, `weights`, `converged`, `convergence.code`, `iter`, `sse`, `variogram.object`), the matrix `param.aniso` with the estimated values of the variogram parameters along with the bounds of the confidence intervals and optionally the correlation matrix `cor.tf.param` of the estimated transformed parameters. There is a `print` method for objects of class `summary.fitted.variogram` which returns invisibly the object unchanged.

The method `lines.fitted.variogram` is called for its side effects and returns the value `NULL` invisibly.

### Author(s)

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## References

Cressie, N. A. C. (1993) *Statistics for Spatial Data*, Wiley, New York, doi:10.1002/9781119115151.

## See Also

[georobPackage](#) for a description of the model and a brief summary of the algorithms; [georob](#) for (robust) fitting of spatial linear models;

[georobObject](#) for a description of the class georob;

[profilelogLik](#) for computing profiles of Gaussian likelihoods;

[plot.georob](#) for display of RE(ML) variogram estimates;

[control.georob](#) for controlling the behaviour of georob;

[georobModelBuilding](#) for stepwise building models of class georob;

[cv.georob](#) for assessing the goodness of a fit by georob;

[georobMethods](#) for further methods for the class georob;

[predict.georob](#) for computing robust Kriging predictions;

[lgpp](#) for unbiased back-transformation of Kriging prediction of log-transformed data;

[georobSimulation](#) for simulating realizations of a Gaussian process from model fitted by georob.

## Examples

```
data(wolfcamp)

## fitting an isotropic IRF(0) model
r.sv.iso <- sample.variogram(pressure~1, data = wolfcamp,
  locations = ~x + y, lag.dist.def = seq(0, 200, by = 15))
plot(r.sv.iso, type = "l")

if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s
  r.irf0.iso <- fit.variogram.model(r.sv.iso, variogram.model = "RMfbm",
    param = c(variance = 100, nugget = 1000, scale = 1., alpha = 1.),
    fit.param = default.fit.param(scale = FALSE, alpha = TRUE))
  summary(r.irf0.iso, correlation = TRUE)
  lines(r.irf0.iso, line.col = "red")
}

## fitting an anisotropic IRF(0) model
r.sv.aniso <- sample.variogram(pressure~1, data = wolfcamp,
  locations = ~x + y, lag.dist.def = seq(0, 200, by = 15),
  xy.angle.def = c(0., 22.5, 67.5, 112.5, 157.5, 180.))
plot(r.sv.aniso, type = "l")

if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s
  r.irf0.aniso <- fit.variogram.model(r.sv.aniso, variogram.model = "RMfbm",
    param = c(variance = 100, nugget = 1000, scale = 1., alpha = 1.5),
    fit.param = default.fit.param(scale = FALSE, alpha = TRUE),
```

```

    aniso = default.aniso(f1 = 0.4, omega = 135.),
    fit.aniso = default.fit.aniso(f1 = TRUE, omega = TRUE),
    control = control.fit.variogram.model(
      maximizer = "optim",
      optim = control.optim(
        method = "BFGS", hessian = TRUE, control = list(maxit = 5000)
      )
    )
  )
  summary(r.irf0.aniso, correlation = TRUE)

  lines(r.irf0.aniso, xy.angle = seq(0, 135, by = 45))
}

```

gencorr

*Variogram Models***Description**

The function `gencorr` computes intrinsic or stationary isotropic generalized correlations (= negative semi-variances computed with sill (variance) parameter equal to 1) for a set of basic variogram models formerly made available by the function `RFfctn` of the now archived R package **Random-Fields**.

**Usage**

```
gencorr(x, variogram.model, param)
```

**Arguments**

<code>x</code>	a numeric vector with scaled lag distances, i.e. lag distances divided by the range parameter <code>param["scale"]</code> .
<code>variogram.model</code>	a character keyword defining the variogram model. Currently, the following models are implemented: "RMaskey", "Rmbessel", "RMcauchy", "RMcircular", "RMcubic", "RMDagum", "RMDampedcos", "RMdewijsian", "RMexp" (default), "RMfbm", "RMgauss", "RMgencauchy", "RMgenfbm", "RMgengneiting", "RMgneiting", "RMlgd", "RMmatern", "RMpenta", "RMqexp", "RMspheric", "RMstable", "RMwave", "RMwhittle", see <i>Details</i> .
<code>param</code>	a named numeric vector with values of the additional parameters of the variogram models such as the smoothness parameter of the Whittle-Matérn model, see <a href="#">param.names</a> for the names of these parameters. Note that some variogram models (e.g. "RMcircular") do not have any additional parameters.

## Details

The name and parametrization of the variogram models originate from the function `RFfctn` of **RandomFields**. The equations and further information are taken (with minor modifications) from the help pages of the respective functions of the archived **R** package **RandomFields**, version 3.3.14 (Schlather et al., 2022). Note that the variance (sill, `param["variance"]`) and the range parameters (`param["scale"]`) are assumed to be equal to 1 in the following formulae, and  $x$  is the lag distance. The variogram functions are stationary and are valid for any number of dimensions if not mentioned otherwise.

The following intrinsic or stationary isotropic variogram functions  $\gamma(x)$  are implemented in `gencorr`:

- `RMaskey`

$$\gamma(x) = 1 - (1 - x)^\alpha 1_{[0,1]}(x)$$

$1_{[0,1]}(x)$  is the indicator function equal to 1 for  $x \in [0, 1]$  and 0 otherwise. This variogram function is valid for dimension  $d$  if  $\alpha \geq (d + 1)/2$ . For  $\alpha = 1$  we get the well-known triangle (or tent) model, which is only valid on the real line.

- `RMbessel`

$$\gamma(x) = 1 - 2^\nu \Gamma(\nu + 1) x^{-\nu} J_\nu(x)$$

where  $\nu \geq \frac{d-2}{2}$ ,  $\Gamma$  denotes the gamma function and  $J_\nu$  is a Bessel function of first kind. This models a hole effect (see *Chilès and Delfiner, 1999, p. 92*). An important case is  $\nu = -0.5$  which gives the variogram function

$$\gamma(x) = 1 - \cos(x)$$

and which is only valid for  $d = 1$  (this equals `RMdampedcos` for  $\lambda = 0$ ). A second important case is  $\nu = 0.5$  with variogram function

$$\gamma(x) = \left(1 - \frac{\sin(x)}{x}\right) 1_{x>0}$$

which is valid for  $d \leq 3$ . This coincides with `RMwave`.

- `RMcauchy`

$$\gamma(x) = 1 - (1 + x^2)^{-\gamma}$$

where  $\gamma > 0$ . The parameter  $\gamma$  determines the asymptotic power law. The smaller  $\gamma$ , the longer the long-range dependence. The generalized Cauchy Family (`RMgencauchy`) includes this family for the choice  $\alpha = 2$  and  $\beta = 2\gamma$ .

- `RMcircular`

$$\gamma(x) = 1 - \left(1 - \frac{2}{\pi} \left(x\sqrt{1-x^2} + \arcsin(x)\right)\right) 1_{[0,1]}(x)$$

This variogram function is valid only for dimensions  $d \leq 2$ .

- `RMcubic`

$$\gamma(x) = 1 - (1 - 7x^2 + 8.75x^3 - 3.5x^5 + 0.75x^7) 1_{[0,1]}(x)$$

The model is only valid for dimensions  $d \leq 3$ . It is a 2 times differentiable variogram function with compact support (see *Chilès and Delfiner, 1999, p. 84*).

- RMdagum

$$\gamma(x) = (1 + x^{-\beta})^{-\gamma/\beta}$$

The parameters  $\beta$  and  $\gamma$  can be varied in the intervals  $(0, 1]$  and  $(0, 1)$ , respectively. Like the generalized Cauchy model (RMgencauchy) the Dagum family can be used to model separately fractal dimension and Hurst effect (see *Berg et al., 2008*).

- RMdampedcos

$$\gamma(x) = 1 - \exp(-\lambda x) \cos(x)$$

The model is valid for any dimension  $d$ . However, depending on the dimension of the random field the following bound  $\lambda \geq 1/\tan(\pi/(2d))$  has to be respected. This variogram function models a hole effect (see *Chilès and Delfiner, 1999, p. 92*). For  $\lambda = 0$  we obtain

$$\gamma(x) = 1 - \cos(x)$$

which is only valid for  $d = 1$  and corresponds to RMbessel for  $\nu = -0.5$ .

- RMdewijsian

$$\gamma(x) = \log(1 + x^\alpha)$$

where  $\alpha \in (0, 2]$ . This is an intrinsic variogram function. Originally, the logarithmic model  $\gamma(x) = \log(x)$  was named after de Wijs and reflects a principle of similarity (see *Chilès and Delfiner, 1999, p. 90*). But note that  $\gamma(x) = \log(x)$  is not a valid variogram function.

- RMexp

$$\gamma(x) = 1 - e^{-x}$$

This model is a special case of the Whittle model (RMwhittle) if  $\nu = 0.5$  and of the stable family (RMstable) if  $\nu = 1$ . Moreover, it is the continuous-time analogue of the first order auto-regressive time series covariance structure.

- RMfbm

$$\gamma(x) = x^\alpha$$

where  $\alpha \in (0, 2)$ . This is an intrinsically stationary variogram function. For  $\alpha = 1$  we get a variogram function corresponding to a standard Brownian Motion. For  $\alpha \in (0, 2)$  the quantity  $H = \frac{\alpha}{2}$  is called Hurst index and determines the fractal dimension  $D = d + 1 - H$  of the corresponding Gaussian sample paths where  $d$  is the dimension of the random field (see *Chilès and Delfiner, 1999, p. 89*).

- RMgauss

$$\gamma(x) = 1 - e^{-x^2}$$

The Gaussian model has an infinitely differentiable variogram function. This smoothness is artificial. Furthermore, this often leads to singular matrices and therefore numerically unstable procedures (see *Stein, 1999, p. 29*). The Gaussian model is included in the stable class (RMstable) for the choice  $\alpha = 2$ .

- RMgencauchy

$$\gamma(x) = 1 - (1 + x^\alpha)^{-\beta/\alpha}$$

where  $\alpha \in (0, 2]$  and  $\beta > 0$ . This model has a smoothness parameter  $\alpha$  and a parameter  $\beta$  which determines the asymptotic power law. More precisely, this model admits simulating random fields where fractal dimension  $D$  of the Gaussian sample path and Hurst coefficient  $H$  can be chosen independently (compare also with RMlgd): Here, we have  $D = d + 1 - \alpha/2$ ,  $\alpha \in (0, 2]$  and  $H = 1 - \beta/2$ ,  $\beta > 0$ . The smaller  $\beta$ , the longer the long-range dependence. The

variogram function is very regular near the origin, because its Taylor expansion only contains even terms and reaches its sill slowly. Note that the Cauchy Family (RMcauchy) is included in this family for the choice  $\alpha = 2$  and  $\beta = 2\gamma$ .

- RMgenfbm

$$\gamma(x) = (1 + x^\alpha)^{\delta/\alpha} - 1$$

where  $\alpha \in (0, 2)$  and  $\delta \in (0, 1)$ . This is an intrinsic variogram function.

- RMgengneiting This is a family of stationary models whose elements are specified by the two parameters  $\kappa$  and  $\mu$  with  $\kappa$  being a non-negative integer and  $\mu \geq \frac{d}{2}$  with  $d$  denoting the dimension of the random field (the models can be used for any dimension). Let  $\beta = \mu + 2\kappa + 1/2$ .

For  $\kappa = 0$  the model equals the Askey model (RMaskey) and is therefore not implemented.

For  $\kappa = 1$  the model is given by

$$\gamma(x) = 1 - (1 + \beta x)(1 - x)^\beta 1_{[0,1]}(x), \quad \beta = \mu + 2.5,$$

If  $\kappa = 2$

$$\gamma(x) = 1 - \left(1 + \beta x + \frac{\beta^2 - 1}{3}x^2\right)(1 - x)^\beta 1_{[0,1]}(x), \quad \beta = \mu + 4.5,$$

and for  $\kappa = 3$

$$\gamma(x) = 1 - \left(1 + \beta x + \frac{(2\beta^2 - 3)}{5}x^2 + \frac{(\beta^2 - 4)\beta}{15}x^3\right)(1 - x)^\beta 1_{[0,1]}(x), \beta = \mu + 6.5,$$

A special case of this family is RMgneiting (with  $s = 1$  there) for the choice  $\kappa = 3, \mu = 3/2$ .

- RMgneiting

$$\gamma(x) = 1 - (1 + 8sx + 25s^2x^2 + 32s^3x^3)(1 - sx)^8$$

if  $0 \leq x \leq \frac{1}{s}$  and

$$\gamma(x) = 1$$

otherwise. Here,  $s = 0.301187465825$ . This variogram function is valid only for dimensions less than or equal to 3. It is 6 times differentiable and has compact support. This model is an alternative to RMgauss as its graph is hardly distinguishable from the graph of the Gaussian model, but possesses neither the mathematical nor the numerical disadvantages of the Gaussian model. It is a special case of RMgengneiting for the choice  $\kappa = 3, \mu = 1.5$ .

- RMLgd

$$\gamma(x) = \frac{\beta}{\alpha + \beta}x^\alpha 1_{[0,1]}(x) + \left(1 - \frac{\alpha}{\alpha + \beta}x^{-\beta}\right)1_{x>1}(x)$$

where  $\beta > 0$  and  $0 < \alpha \leq (3 - d)/2$ , with  $d$  denoting the dimension of the random field. The model is only valid for dimension  $d = 1, 2$ . This model admits simulating random fields where fractal dimension  $D$  of the Gaussian sample and Hurst coefficient  $H$  can be chosen independently (compare also RMgencauchy): Here, the random field has fractal dimension  $D = d + 1 - \alpha/2$  and Hurst coefficient  $H = 1 - \beta/2$  for  $0 < \beta \leq 1$ .

- RMmatern

$$\gamma(x) = 1 - \frac{2^{1-\nu}}{\Gamma(\nu)} (\sqrt{2\nu x})^\nu K_\nu(\sqrt{2\nu x})$$

where  $\nu > 0$  and  $K_\nu$  is the modified Bessel function of second kind. This is one of 3 possible parametrizations (Whittle, Matérn, Handcock-Wallis) of the Whittle-Matérn model. The Whittle-Matérn model is the model of choice if the smoothness of a random field is to be parametrized: the sample paths of a Gaussian random field with this covariance structure are  $m$  times differentiable if and only if  $\nu > m$  (see *Gneiting and Guttorp, 2010, p. 24*). Furthermore, the fractal dimension  $D$  of the Gaussian sample paths is determined by  $\nu$ : We have  $D = d + 1 - \nu, \nu \in (0, 1)$  and  $D = d$  for  $\nu > 1$  where  $d$  is the dimension of the random field (see *Stein, 1999, p. 32*). If  $\nu = 0.5$  the Matérn model equals RMexp. For  $\nu$  tending to  $\infty$  a rescaled Gaussian model RMgauss appears as limit for the Handcock-Wallis parametrization.

- RMpenta

$$\gamma(x) = 1 - \left(1 - \frac{22}{3}x^2 + 33x^4 - \frac{77}{2}x^5 + \frac{33}{2}x^7 - \frac{11}{2}x^9 + \frac{5}{6}x^{11}\right) 1_{[0,1]}(x)$$

The model is only valid for dimensions  $d \leq 3$ . It has a 4 times differentiable variogram function with compact support (cf. *Chilès and Delfiner, 1999, p. 84*).

- RMqexp

$$\gamma(x) = 1 - \frac{2e^{-x} - \alpha e^{-2x}}{2 - \alpha}$$

where  $\alpha \in [0, 1]$ .

- RMspheric

$$\gamma(x) = 1 - \left(1 - \frac{3}{2}x + \frac{1}{2}x^3\right) 1_{[0,1]}(x)$$

This variogram model is valid only for dimensions less than or equal to 3 and has compact support.

- RMstable

$$\gamma(x) = 1 - e^{-x^\alpha}$$

where  $\alpha \in (0, 2]$ . The parameter  $\alpha$  determines the fractal dimension  $D$  of the Gaussian sample paths:  $D = d + 1 - \alpha/2$  where  $d$  is the dimension of the random field. For  $\alpha < 2$  the Gaussian sample paths are not differentiable (see *Gelfand et al., 2010, p. 25*). The stable family includes the exponential model (RMexp) for  $\alpha = 1$  and the Gaussian model (RMgauss) for  $\alpha = 2$ .

- RMwave

$$\gamma(x) = \left(1 - \frac{\sin(x)}{x}\right) 1_{x>0}$$

The model is only valid for dimensions  $d \leq 3$ . It is a special case of RMbessel for  $\nu = 0.5$ . This variogram models a hole effect (see *Chilès and Delfiner, 1999, p. 92*).

- RMwhittle

$$\gamma(x) = 1 - \frac{2^{1-\nu}}{\Gamma(\nu)} x^\nu K_\nu(x)$$

where  $\nu > 0$  and  $K_\nu$  is the modified Bessel function of second kind. This is one of 3 possible parametrizations (Whittle, Matérn, Handcock-Wallis) of the Whittle-Matérn model, for further details, see information for entry RMmatern above.



**Value**

A numeric vector with generalized correlations (= negative semi-variances computed with variance parameter `param["variance"] = 1`).

**Author(s)**

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**References**

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**See Also**

[georobPackage](#) for a description of the model and a brief summary of the algorithms;

[georob](#) for (robust) fitting of spatial linear models;

[georobObject](#) for a description of the class `georob`;

[profilelogLik](#) for computing profiles of Gaussian likelihoods;

[plot.georob](#) for display of RE(ML) variogram estimates;

[control.georob](#) for controlling the behaviour of `georob`;

[georobModelBuilding](#) for stepwise building models of class `georob`;

[cv.georob](#) for assessing the goodness of a fit by `georob`;

[georobMethods](#) for further methods for the class `georob`;

[predict.georob](#) for computing robust Kriging predictions;

[lgnp](#) for unbiased back-transformation of Kriging prediction of log-transformed data;

[georobSimulation](#) for simulating realizations of a Gaussian process from model fitted by `georob`; and finally

`sample.variogram` and `fit.variogram.model` for robust estimation and modelling of sample variograms.

### Examples

```
## scaled lag distances
x <- seq(0, 3, length.out = 100)

## generalized correlations stable model
y <- gencorr(x, variogram.model = "RMstable", param = c(alpha = 1.5))
plot(x, y)

## generalized correlations circular model
y <- gencorr(x, variogram.model = "RMcircular")
plot(x, y)
```

---

georob

*Robust Fitting of Spatial Linear Models*

---

### Description

The function `georob` fits a linear model with spatially correlated errors to geostatistical data that are possibly contaminated by independent outliers. The regression coefficients and the parameters of the variogram model are estimated by robust or Gaussian restricted maximum likelihood (REML) or by Gaussian maximum likelihood (ML).

### Usage

```
georob(formula, data, subset, weights, na.action, model = TRUE,
       x = FALSE, y = FALSE, contrasts = NULL, offset, locations,
       variogram.model = c("RMexp", "RMaskey", "RMbessel", "RMcauchy",
                           "RMcircular", "RMcubic", "RMDagum", "RMDampedcos", "RMDewijsian",
                           "RMfbm", "RMgauss", "RMgencauchy", "RMgenfbm", "RMgengneiting",
                           "RMgneiting", "RMLgd", "RMmatern", "RMpenta", "RMqexp",
                           "RMspheric", "RMstable", "RMwave", "RMwhittle"),
       param, fit.param = default.fit.param()[names(param)],
       aniso = default.aniso(), fit.aniso = default.fit.aniso(),
       variogram.object = NULL,
       tuning.psi = 2, control = control.georob(),
       verbose = 0, ...)
```

### Arguments

<code>formula</code>	a symbolic description of the regression model for the external drift to be fit (mandatory argument). See <code>lm</code> and <code>formula</code> for more details.
<code>data</code>	an optional data frame, a <code>SpatialPointsDataFrame</code> , list or environment (or another object coercible by <code>as.data.frame</code> to a data frame) containing the variables in the model and the coordinates where the data was recorded. If not

	found in data, the variables are taken from <code>environment(formula)</code> , typically the environment from which <code>georob</code> is called.
<code>subset</code>	an optional vector specifying a subset of observations to be used in the fitting process.
<code>weights</code>	an optional vector of weights to be used in the fitting process, currently ignored.
<code>na.action</code>	a function which indicates what should happen when the data contain NAs. The default is set by the <code>na.action</code> argument of <code>options</code> , and is <code>na.fail</code> if that is unset. The “factory-fresh” default is <code>na.omit</code> . Another possible value is <code>NULL</code> , no action. Value <code>na.exclude</code> can be useful.
<code>model, x, y</code>	logical scalars. If <code>TRUE</code> the corresponding components of the fit (the model frame, the model matrix, the response) are returned. The model frame is augmented by the coordinates.
<code>contrasts</code>	an optional list. See the <code>contrasts.arg</code> of <code>model.matrix.default</code> .
<code>offset</code>	this optional argument can be used to specify an <i>a priori</i> known component to be included in the linear predictor during fitting. An <code>offset</code> term can be included in the formula instead or as well, and if both are specified their sum is used.
<code>locations</code>	a one-sided formula defining the variables that are used as coordinates of the locations where the data was recorded (mandatory argument).
<code>variogram.model</code>	a character keyword defining the variogram model to be fitted. Currently, most basic variogram models provided formerly by the now archived package <b>RandomFields</b> can be fitted (see <i>Details</i> and <code>gencorr</code> ).
<code>param</code>	a named numeric vector with initial values of the variogram parameters (mandatory argument). The names of <code>param</code> are matched against the following names (see <i>Details</i> and <code>georobPackage</code> for information about the parametrization of variogram models): <ul style="list-style-type: none"> <li>• <code>variance</code>: variance (sill <math>\sigma^2</math>) of the auto-correlated component of the Gaussian random field <math>B(s)</math>.</li> <li>• <code>snugget</code>: variance (spatial nugget <math>\sigma_n^2</math>) of the seemingly spatially uncorrelated component of <math>B(s)</math> (micro-scale spatial variation; default value <code>snugget = 0</code>).</li> <li>• <code>nugget</code>: variance (nugget <math>\tau^2</math>) of the independent errors <math>\varepsilon(s)</math>.</li> <li>• <code>scale</code>: range parameter (<math>\alpha</math>) of the variogram.</li> <li>• names of additional variogram parameters such as the smoothness parameter <math>\nu</math> of the Whittle-Matérn model (see <code>gencorr</code> and <code>param.names</code>).</li> </ul>
<code>fit.param</code>	a named logical vector (or a function such as <code>default.fit.param</code> that creates this vector) with the same names as used for <code>param</code> , defining which parameters are adjusted ( <code>TRUE</code> ) and which are kept fixed at their initial values ( <code>FALSE</code> ) when fitting the model.
<code>aniso</code>	a named numeric vector with initial values (or a function such as <code>default.aniso</code> that creates this vector) for fitting geometrically anisotropic variogram models. The names of <code>aniso</code> are matched against the following names (see <i>Details</i> and <code>georobPackage</code> for information about the parametrization of variogram models):

- $f_1$ : ratio  $f_1$  of lengths of second and first semi-principal axes of an ellipsoidal surface with constant semi-variance in  $\mathbb{R}^3$  (default  $f_1 = 1$ ).
- $f_2$ : ratio  $f_2$  of lengths of third and first semi-principal axes of the semi-variance ellipsoid (default  $f_2 = 1$ ).
- $\omega$ : azimuth in degrees of the first semi-principal axis of the semi-variance ellipsoid (default  $\omega = 90$ ).
- $\phi$ : 90 degrees minus latitude of the first semi-principal axis of the semi-variance ellipsoid (default  $\phi = 90$ ).
- $\zeta$ : angle in degrees between the second semi-principal axis and the direction of the line defined by the intersection between the  $x$ - $y$ -plane and the plane orthogonal to the first semi-principal axis of the semi-variance ellipsoid through the origin (default  $\zeta = 0$ ).

`fit.aniso` a named logical vector (or a function such as `default.fit.aniso` that creates this vector) with the same names as used for `aniso`, defining which parameters are adjusted (TRUE) and which are kept fixed at their initial values (FALSE) when fitting the model.

`variogram.object` an optional list that defines a possibly nested variogram model. Each component is itself a list with the following components:

- `variogram.model`: a mandatory character keyword defining the variogram model, see respective argument above.
- `param`: a mandatory named numeric vector with initial values of the variogram parameters, see respective argument above.
- `fit.param`: an optional named logical vector defining which parameters are adjusted, see respective argument above.
- `aniso`: an optional named numeric vector with initial values for fitting geometrically anisotropic variogram models, see respective argument above.
- `fit.param`: an optional named logical vector defining which anisotropy parameters are adjusted, see respective argument above.

Note that the arguments `variogram.model`, `param`, `fit.param`, `aniso` and `fit.aniso` are ignored when `variogram.object` is passed to `georob`.

`tuning.psi` positive numeric. The tuning constant  $c$  of the  $\psi_c$ -function of the robust REML algorithm.

`control` a list specifying parameters that control the behaviour of `georob`. Use the function `control.georob` and see its help page for the components of `control`.

`verbose` positive integer controlling logging of diagnostic messages to the console during model fitting. `verbose = 0` largely suppresses such messages and `verbose = 4` asks for most verbose output (see `control` arguments of `nleqslv`, `nlminb` and `optim` and `control.georob` for information how to fine tuning diagnostic output generated by `nleqslv`, `nlminb` and `optim`).

... further arguments passed to function (e.g. `object`. used internally for updating `georob` objects).

## Details

georob fits a spatial linear model by robust (Künsch *et al.*, 2011, Künsch *et al.*, in preparation) or Gaussian RE(ML) (Harville, 1977). [georobPackage](#) describes the employed model and briefly sketches the robust REML estimation and the robust external drift Kriging method. Here, we describe further details of georob.

### Implemented variograms:

Currently, most basic variogram models provided formerly by the now archived package **RandomFields** can be fitted by georob (see argument `variogram.model` and [gencorr](#) for a list of implemented models). Some of these models have in addition to variance, `snugget`, `nugget` and `scale` further parameters. Initial values of these parameters (`param`) and fitting flags (`fit.param`) must be passed to georob by the same names as used for the models RM... in [gencorr](#). Use the function [param.names](#) to list additional parameters of a given `variogram.model`.

The arguments `fit.param` and `fit.aniso` are used to control what variogram and anisotropy parameters are estimated and which are kept at the constant initial values. The functions [default.fit.param](#) and [default.fit.aniso](#) set reasonable default values for these arguments. Note, as an aside, that the function [default.aniso](#) sets (default) values of the anisotropy parameters for an isotropic variogram.

### Estimating parameters of power function variogram:

The intrinsic variogram model `RMfbm` is over-parametrized when both the variance (plus possibly `snugget`) and the `scale` are estimated. Therefore, to estimate the parameters of this model, `scale` must be kept fixed at an arbitrary value by using `fit.param["scale"] = FALSE`.

### Estimating parameters of geometrically anisotropic variograms:

The subsection **Model** of [georobPackage](#) describes how such models are parametrized and gives definitions the various elements of `aniso`. Some additional remarks might be helpful:

- The first semi-principal axis points into the direction with the farthest reaching auto-correlation, which is described by the range parameter `scale` ( $\alpha$ ).
- The ranges in the direction of the second and third semi-principal axes are given by  $f_1\alpha$  and  $f_2\alpha$ , with  $0 < f_2 \leq f_1 \leq 1$ .
- The default values for `aniso` ( $f_1 = 1$ ,  $f_2 = 1$ ) define an isotropic variogram model.
- Valid ranges for the angles characterizing the orientation of the semi-variance ellipsoid are (in degrees):  $\omega$   $[0, 180]$ ,  $\phi$   $[0, 180]$ ,  $\zeta$   $[-90, 90]$ .

### Estimating variance of micro-scale variation:

Simultaneous estimation of the variance of the micro-scale variation (`snugget`,  $\sigma_n^2$ ), appears seemingly as spatially uncorrelated with a given sampling design, and of the variance (`nugget`,  $\tau^2$ ) of the independent errors requires that for some locations  $s_i$  replicated observations are available. Locations less or equal than `zero.dist` apart are thereby considered as being coincident (see [control.georob](#)).

### Constraining estimates of variogram parameters:

Parameters of variogram models can vary only within certain bounds (see [param.bounds](#) and [gencorr](#) for allowed ranges). georob uses three mechanisms to constrain parameter estimates to permissible ranges:

1. *Parameter transformations*: By default, all variance (variance, snugget, nugget), the range scale, the anisotropy parameters f1 and f2 and many of the additional parameters are log-transformed before solving the estimating equations or maximizing the restricted log-likelihood and this warrants that the estimates are always positive (see `control.georob` for detailed explanations how to control parameter transformations).
2. *Checking permissible ranges*: The additional parameters of the variogram models such as the smoothness parameter  $\nu$  of the Whittle-Matérn model are forced to stay in the permissible ranges by signalling an error to `nleqslv`, `nlminb` or `optim` if the current trial values are invalid. These functions then graciously update the trial values of the parameters and carry their task on. However, it is clear that such a procedure likely gets stuck at a point on the boundary of the parameter space and is therefore just a workaround for avoiding runtime errors due to invalid parameter values.
3. *Exploiting the functionality of nlminb and optim*: If a spatial model is fitted non-robustly, then the arguments `lower`, `upper` (and method of `optim`) can be used to constrain the parameters (see `control.optim` how to pass them to `optim`). For `optim` one has to use the arguments `method = "L-BFGS-B"`, `lower = l`, `upper = u`, where `l` and `u` are numeric vectors with the lower and upper bounds of the *transformed* parameters in the order as they appear in `c(variance, snugget, nugget, scale, ...)[fit.param]`, `aniso[fit.aniso]`, where `...` are additional parameters of isotropic variogram models (use `param.names(variogram.model)` to display the names and the order of the additional parameters for `variogram.model`). For `nlminb` one has to use the arguments `lower = l`, `upper = u`, where `l` and `u` are numeric vectors as described above.

#### Computing robust initial estimates of parameters for robust REML:

To solve the robustified estimating equations for  $B$  and  $\beta$  the following initial estimates are used:

- $\hat{B} = \mathbf{0}$ , if this turns out to be infeasible, initial values can be passed to `georob` by the argument `bhat` of `control.georob`.
- $\hat{\beta}$  is either estimated robustly by the function `lmrob`, `rq` or non-robustly by `lm` (see argument `initial.fixef` of `control.georob`).

Finding the roots of the robustified estimating equations of the variogram and anisotropy parameters is more sensitive to a good choice of initial values than maximizing the Gaussian (restricted) log-likelihood with respect to the same parameters. If the initial values for `param` and `aniso` are not sufficiently close to the roots of the system of nonlinear equations, then `nleqslv` may fail to find them. Setting `initial.param = TRUE` (see `control.georob`) allows one to find initial values that are often sufficiently close to the roots so that `nleqslv` converges. This is achieved by:

1. Initial values of the regression parameters are computed by `lmrob` irrespective of the choice for `initial.fixef` (see `control.georob`).
2. Observations with “robustness weights” of the `lmrob` fit, satisfying  $\psi_c(\hat{\varepsilon}_i/\hat{\tau})/(\hat{\varepsilon}_i/\hat{\tau}) \leq \text{min.rweight}$ , are discarded (see `control.georob`).
3. The model is fit to the pruned data set by Gaussian REML using `nlminb` or `optim`.
4. The resulting estimates of the variogram parameters (`param`, `aniso`) are used as initial estimates for the subsequent robust fit of the model by `nleqslv`.

Note that for step 3 above, initial values of `param` and `aniso` must be provided to `georob`.

#### Estimating variance parameters by Gaussian (RE)ML:

Unlike robust REML, where robustified estimating equations are solved for the variance parameters `nugget` ( $\tau^2$ ), `variance` ( $\sigma^2$ ), and possibly `snugget` ( $\sigma_n^2$ ), for Gaussian (RE)ML the variances can be re-parametrized to

- the signal variance  $\sigma_B^2 = \sigma^2 + \sigma_n^2$ ,
- the inverse relative nugget  $\eta = \sigma_B^2/\tau^2$  and
- the relative auto-correlated signal variance  $\xi = \sigma^2/\sigma_B^2$ .

georob maximizes then a (restricted) *profile log-likelihood* that depends only on  $\eta$ ,  $\xi$ ,  $\alpha$ , ..., and  $\sigma_B^2$  is estimated by an explicit expression that depends on these parameters (e.g. *Diggle and Ribeiro, 2006, p. 113*). This is usually more efficient than maximizing the (restricted) log-likelihood with respect to the original variance parameters  $\tau^2$ ,  $\sigma_n^2$  and  $\sigma^2$ . georob chooses the parametrization automatically, but the user can control it by the argument `reparam` of the function `control.georob`.

### Value

An object of class `georob` representing a robust (or Gaussian) (RE)ML fit of a spatial linear model. See `georobObject` for the components of the fit.

### Author(s)

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with contributions by Cornelia Schwierz.

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### See Also

`georobPackage` for a description of the model and a brief summary of the algorithms;  
`georobObject` for a description of the class `georob`;  
`profilelogLik` for computing profiles of Gaussian likelihoods;  
`plot.georob` for display of RE(ML) variogram estimates;  
`control.georob` for controlling the behaviour of `georob`;  
`georobModelBuilding` for stepwise building models of class `georob`;  
`cv.georob` for assessing the goodness of a fit by `georob`;  
`georobMethods` for further methods for the class `georob`;  
`predict.georob` for computing robust Kriging predictions;  
`lgnpp` for unbiased back-transformation of Kriging prediction of log-transformed data;

`georobSimulation` for simulating realizations of a Gaussian process from model fitted by `georob`; and finally

`sample.variogram` and `fit.variogram.model` for robust estimation and modelling of sample variograms.

## Examples

```
#####
## meuse data ##
#####
data(meuse)

## Gaussian REML fit
r.logzn.reml <- georob(log(zinc) ~ sqrt(dist), data = meuse, locations = ~ x + y,
  variogram.model = "RMexp",
  param = c(variance = 0.15, nugget = 0.05, scale = 200),
  tuning.psi = 1000)
summary(r.logzn.reml, correlation = TRUE)
plot(r.logzn.reml, lag.dist.def = seq(0, 2000, by = 100))

## robust REML fit
if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s
  r.logzn.rob <- update(r.logzn.reml, tuning.psi = 1)

  summary(r.logzn.rob, correlation = TRUE)
  lines(r.logzn.rob, col = "red")
}

#####
## wolfcamp data ##
#####
data(wolfcamp)

## fitting isotropic IRF(0) model

r.irf0.iso <- georob(pressure ~ 1, data = wolfcamp, locations = ~ x + y,
  variogram.model = "RMfbm",
  param = c(variance = 10, nugget = 1500, scale = 1, alpha = 1.5),
  fit.param = default.fit.param(scale = FALSE, alpha = TRUE),
  tuning.psi = 1000)

summary(r.irf0.iso)
plot(r.irf0.iso, lag.dist.def = seq(0, 200, by = 7.5))

## fitting anisotropic IRF(0) model
if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s
  r.irf0.aniso <- georob(pressure ~ 1, data = wolfcamp, locations = ~ x + y,
    variogram.model = "RMfbm",
    param = c(variance = 5.9, nugget = 1450, scale = 1, alpha = 1),
```



```

    fit.param = default.fit.param(scale = FALSE, alpha = TRUE),
    aniso = default.aniso(f1 = 0.51, omega = 148.),
    fit.aniso = default.fit.aniso(f1 = TRUE, omega = TRUE),
    tuning.psi = 1000)
summary(r.irf0.aniso)
plot(r.irf0.aniso, lag.dist.def = seq(0, 200, by = 7.5),
     xy.angle.def = c(0, 22.5, 67.5, 112.5, 157.5, 180.),
     add = TRUE, col = 2:5)

  pchisq(2*(r.irf0.aniso[["loglik"]] - r.irf0.iso[["loglik"]]), 2, lower = FALSE)
}

```

---

georobModelBuilding    *S3 Methods for Stepwise Building Fixed-Effects Models for Class*  
georob

---

## Description

This page documents the methods `deviance`, `logLik`, `extractAIC`, `add1`, `drop1`, `step` and `waldtest` for the class `georob`. The package `georob` provides a generic `step` function and a default method which is identical with the (non-generic) function `step`.

## Usage

```

## S3 method for class 'georob'
deviance(object, warn = TRUE, REML = FALSE, ...)

## S3 method for class 'georob'
logLik(object, warn = TRUE, REML = FALSE, ...)

## S3 method for class 'georob'
extractAIC(fit, scale = 0, k = 2, ...)

## S3 method for class 'georob'
add1(object, scope, scale = 0, test = c("none", "Chisq"), k = 2,
     trace = FALSE, fixed = TRUE, use.fitted.param = TRUE, verbose = 0,
     ncores = 1, ...)

## S3 method for class 'georob'
drop1(object, scope, scale = 0, test = c("none", "Chisq"), k = 2,
     trace = FALSE, fixed = TRUE, use.fitted.param = TRUE, verbose = 0,
     ncores = 1, ...)

step(object, ...)

## Default S3 method:
step(object, scope, scale = 0,
     direction = c("both", "backward", "forward"), trace = 1,

```

```

keep = NULL, steps = 1000, k = 2, ...)

## S3 method for class 'georob'
step(object, scope, scale = 0,
      direction = c("both", "backward", "forward"), trace = 1,
      keep = NULL, steps = 1000, k = 2,
      fixed.add1.drop1 = TRUE, fixed.step = fixed.add1.drop1,
      use.fitted.param = TRUE, verbose = 0, ncores = 1, ...)

## S3 method for class 'georob'
waldtest(object, ..., vcov = NULL, test = c("F", "Chisq"),
          name = NULL)

```

## Arguments

object, fit	an object of class georob, see <a href="#">georobObject</a> .
direction	a character keyword with the mode of stepwise search, see <a href="#">step</a> .
fixed, fixed.add1.drop1	a logical scalar controlling whether the variogram parameters are <i>not</i> adjusted when adding or dropping model terms by add1 and drop1 (default TRUE), see <a href="#">Details</a> .
fixed.step	a logical scalar controlling whether the variogram parameters are <i>not</i> adjusted after having called add1 and drop1 in step (default TRUE), see <a href="#">Details</a> .
k	a numeric specifying the 'weight' of the equivalent degrees of freedom (=: edf) part in the AIC formula, see <a href="#">extractAIC</a> .
keep	a filter function whose input is a fitted model object and the associated AIC statistic, and whose output is arbitrary, see <a href="#">step</a> .
name	a function for extracting a suitable name/description from a fitted model object. By default the name is queried by calling <a href="#">formula</a> , see <a href="#">waldtest</a> .
ncores	an integer specifying the number of cores used for parallelized execution of add1 and drop1. If larger than one then the minimum of ncores, <code>parallel::detectCores()</code> and the number of terms to be added or dropped determines the number of cores that is actually used.
REML	a logical scalar controlling whether the restricted log-likelihood should be extracted (default TRUE).
scale	a numeric, currently not used, see <a href="#">extractAIC</a> .
scope	defines the range of models examined in the stepwise search. This should be either a single formula, or a list containing components upper and lower, both formulae, see <a href="#">step</a> for details.
steps	a numeric with the maximum number of steps to be considered (default is 1000), see <a href="#">step</a> .
test	a character keyword specifying whether to compute the large sample Chi-squared statistic (with asymptotic Chi-squared distribution) or the finite sample F statistic (with approximate F distribution), see <a href="#">waldtest</a> .

trace	a numeric. If positive, information is printed during the running of step, see <a href="#">step</a> .
use.fitted.param	a logical scalar controlling whether fitted values of param (and aniso are used as initial values when variogram parameters are fitted afresh for adding and dropping terms from the model (default TRUE). If equal to FALSE then the initial values in object[["call"]] are used.
vcov	a function for estimating the covariance matrix of the regression coefficients, see <a href="#">waldtest</a> .
verbose	a positive integer controlling logging of diagnostic messages to the console during model fitting, see <a href="#">georob</a> (default 0).
warn	a logical scalar controlling whether warnings should be suppressed.
...	additional arguments passed to methods (see in particular <code>waldtest.default</code> ).

## Details

For a non-robust fit the function deviance returns the residual deviance

$$(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})^T (\hat{\tau}^2 \mathbf{I} + \boldsymbol{\Gamma}_{\hat{\theta}})^{-1} (\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}})$$

(see [georobPackage](#) for an explanation of the notation). For a robust fit the deviance is not defined. The function then computes with a warning the deviance of an equivalent Gaussian model with heteroscedastic nugget  $\tau^2/w$  where  $w$  are the “robustness weights” `rweights`, see [georobObject](#).

`logLik` returns the maximized (restricted) log-likelihood. For a robust fit, the log-likelihood is not defined. The function then computes the (restricted) log-likelihood of an equivalent Gaussian model with heteroscedastic nugget (see above).

The methods `extractAIC`, `add1`, `drop1` and `step` are used for stepwise model building.

If `fixed=TRUE` or `fixed.add1.drop1=TRUE` (default) then the variogram parameters are kept fixed at the values of `object`. For `fixed=FALSE` or `fixed.add1.drop1=FALSE` the variogram parameters are fitted afresh for each model tested by `add1` and `drop1`. Then either the variogram parameters in `object$initial.objects` (`use.fitted.param=FALSE`) or the fitted parameters of `object` (`use.fitted.param=TRUE`) are used as initial values. For `fixed.step=TRUE` the variogram parameters are *not* fitted afresh by step after the calls to `drop1` and `add1` have been completed, unlike for `fixed.step=FALSE` where the parameters are estimated afresh for the new model that minimized AIC (BIC) in the previous step.

In addition, the functions of the R package **multcomp** can be used to test general linear hypotheses about the fixed effects of the model.

## Value

The method `deviance.georob` returns the deviance of the fitted spatial linear model with the attributes `log.det.covmat` containing the logarithm of the determinant of the covariance matrix  $\tau^2 \mathbf{I} + \boldsymbol{\Gamma}_{\theta}$  of the observations and optionally `log.det.xticovmatx` with the logarithm of the determinant of  $\mathbf{X}^T (\tau^2 \mathbf{I} + \boldsymbol{\Gamma}_{\theta})^{-1} \mathbf{X}$ , when `REML = true`, see *Details* above.

The method `logLik.georob` returns an object of class `logLik` with the maximized (restricted) log-likelihood, see *Details* above and [logLik](#).

The method `extractAIC.georob` returns a numeric vector of length 2 with the first and second elements giving the equivalent degrees of freedom and the (generalized) Akaike Information Criterion for the fitted model fit.

The methods `add1.georob` and `drop1.georob` return objects of class `anova` which are `data.frames` summarizing the differences in fit between models. In addition to the customary variables `Df` and `AIC` the output contains a logical variable `Converged` which signals (non-)convergence when fitting the respective sub-model.

The generic function `step` returns the stepwise selected model plus optionally some additional attributes depending on the method.

The methods `step.default` and `step.georob` return the stepwise-selected model with up to two additional components (`anova`, `keep`), see [step](#) for details.

The method `waldtest.georob` returns an object of class `anova` which contains the residual degrees of freedom, the difference in degrees of freedom, Wald statistic (either "Chisq" or "F") and corresponding *p*-value.

### Author(s)

Andreas Papritz <papritz@retired.ethz.ch>.

### See Also

[georobPackage](#) for a description of the model and a brief summary of the algorithms;  
[georob](#) for (robust) fitting of spatial linear models;  
[georobObject](#) for a description of the class `georob`;  
[profilelogLik](#) for computing profiles of Gaussian likelihoods;  
[plot.georob](#) for display of RE(ML) variogram estimates;  
[control.georob](#) for controlling the behaviour of `georob`;  
[cv.georob](#) for assessing the goodness of a fit by `georob`;  
[georobMethods](#) for further methods for the class `georob`;  
[predict.georob](#) for computing robust Kriging predictions;  
[lgpp](#) for unbiased back-transformation of Kriging prediction of log-transformed data;  
[georobSimulation](#) for simulating realizations of a Gaussian process from model fitted by `georob`;  
 and finally  
[sample.variogram](#) and [fit.variogram.model](#) for robust estimation and modelling of sample variograms.

### Examples

```
data(meuse)

## Gaussian REML fit
r.logzn.reml <- georob(log(zinc) ~ sqrt(dist), data = meuse, locations = ~ x + y,
  variogram.model = "RMexp",
  param = c(variance = 0.15, nugget = 0.05, scale = 200),
  tuning.psi = 1000)
```

```

summary(r.logzn.reml, correlation = TRUE)

deviance(r.logzn.reml)
logLik(r.logzn.reml)

waldtest(r.logzn.reml, .~. + ffreq)

step(r.logzn.reml, ~ sqrt(dist) + ffreq + soil)

## robust REML fit
if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s

  r.logzn.rob <- update(r.logzn.reml, tuning.psi = 1)

  deviance(r.logzn.rob)
  logLik(r.logzn.rob)
  logLik(r.logzn.rob, REML=TRUE)

  step(r.logzn.rob, ~ sqrt(dist) + ffreq + soil, fixed.step=FALSE, trace=2)
}

```

---

georobObject

*Fitted georob Object*


---

## Description

An object of class `georob` as returned by `georob` and representing a (robustly) fitted spatial linear model. Objects of this class have methods for model building (see `georobModelBuilding`) and cross-validation (see `cv.georob`), for computing (robust) Kriging predictions (see `predict.georob`), for plotting (see `plot.georob`) and for common generic functions (see `georobMethods`).

## Value

A `georob` object is a list with following components:

<code>loglik</code>	the maximized (restricted) Gaussian log-likelihood of a non-robust (RE)ML fit or NA for a robust fit if <code>tuning.psi</code> is less than <code>tuning.psi.nr</code> .
<code>variogram.object</code>	the estimated parameters of a possibly nested variograms model. This is a list that contains for each variogram model structure the following components: <ul style="list-style-type: none"> <li><code>variogram.model</code>: the name of the fitted parametric variogram model.</li> <li><code>param</code>: a named numeric vector with the (estimated) variogram parameters.</li> <li><code>fit.param</code>: a named logical vector with the flags defining what variogram parameters were estimated.</li> <li><code>isotropic</code>: logical indicating whether an isotropic variogram was fitted.</li> <li><code>aniso</code>: a named numeric vector with the (estimated) anisotropy parameters.</li> </ul>

	<ul style="list-style-type: none"> <li>• <code>fit.aniso</code>: a named logical vector with the flags defining what anisotropy parameters were estimated.</li> <li>• <code>sincos</code>: a list with <code>sin</code> and <code>cos</code> of the angles <math>\omega</math>, <math>\phi</math> and <math>\zeta</math> that define the orientation of the anisotropy ellipsoid (see <a href="#">georobPackage</a>).</li> <li>• <code>rotmat</code>: the matrix <math>(C_1, C_2, C_3)</math> (see <a href="#">georobPackage</a>).</li> <li>• <code>sclmat</code>: a vector with the elements <math>1, 1/f_1, 1/f_2</math> (see <a href="#">georobPackage</a>).</li> </ul>
<code>gradient</code>	a named numeric vector with the estimating equations (robust REML) or the gradient of the maximized (restricted) log-likelihood (Gaussian (RE)ML) evaluated at the solution.
<code>tuning.psi</code>	the value of the tuning constant $c$ of the $\psi_c$ -function.
<code>coefficients</code>	a named vector with the estimated regression coefficients $\hat{\beta}$ .
<code>fitted.values</code>	a named vector with the fitted values of the external drift $X\hat{\beta}$ .
<code>bhat</code>	a named vector with the predicted spatial random effects $\hat{B}$ at the data locations.
<code>residuals</code>	a named vector with the residuals $\hat{\varepsilon} = Y - X\hat{\beta} - \hat{B}$ .
<code>rweights</code>	a named numeric vector with the “robustness weights” $\psi_c(\hat{\varepsilon}_i/\hat{\tau})/(\hat{\varepsilon}_i/\hat{\tau})$ .
<code>converged</code>	a logical scalar indicating whether numerical maximization of the (restricted) log-likelihood by <code>nlminb</code> or <code>optim</code> or root finding by <code>nleqslv</code> converged.
<code>convergence.code</code>	a diagnostic integer issued by <code>nlminb</code> , <code>optim</code> (component convergence) or <code>nleqslv</code> (component termcd) about convergence.
<code>iter</code>	a named integer vector of length two, indicating either <ul style="list-style-type: none"> <li>• the number of function and gradient evaluations when maximizing the (restricted) Gaussian log-likelihood by <code>nlminb</code> or <code>optim</code>, or</li> <li>• the number of function and Jacobian evaluations when solving the robustified estimating equations by <code>nleqslv</code>.</li> </ul>
<code>Tmat</code>	the compressed design matrix for replicated observations at coincident locations (integer vector that contains for each observation the row index of the respective unique location).
<code>cov</code>	a list with covariance matrices (or diagonal variance vectors). Covariance matrices are stored in <i>compressed form</i> (see <a href="#">compress</a> ) and can be expanded to square matrices by <a href="#">expand</a> . What <code>cov</code> actually contains depends on the flags passed to <code>georob</code> for computing covariances (see <a href="#">control.georob</a> ). Possible components are: <ul style="list-style-type: none"> <li>• <code>cov.bhat</code>: the covariances of <math>\hat{B}</math>.</li> <li>• <code>cov.betahat</code>: the covariances of <math>\hat{\beta}</math>.</li> <li>• <code>cov.delta.bhat</code>: the covariances of <math>B - \hat{B}</math>.</li> <li>• <code>cov.delta.bhat.betahat</code>: the covariances of <math>B - \hat{B}</math> and <math>\hat{\beta}</math>.</li> <li>• <code>cov.ehat</code>: the covariances of <math>\hat{\varepsilon} = Y - X\hat{\beta} - \hat{B}</math>.</li> <li>• <code>cov.ehat.p.bhat</code>: the covariances of <math>\hat{\varepsilon} + \hat{B} = Y - X\hat{\beta}</math>.</li> <li>• <code>cov.pred.target</code>: a covariance term required for the back-transformation of Kriging predictions of log-transformed data.</li> </ul>

expectations	a named numeric vector with the expectations of $\partial\psi_c(x)/\partial x$ and $\psi_c^2(x)$ with respect to a standard normal distribution ( <code>exp.gauss.dpsi</code> , <code>var.gauss.psi</code> ) and the expectations of $\varepsilon^2$ and $\psi_c^2(x)$ with respect to the long-tailed distribution of $\varepsilon$ ( <code>var.f0.eps</code> , <code>var.f0.psi</code> ).
Valphaxi.objects	a list of matrices in <i>compressed form</i> with (among others) the following components: <ul style="list-style-type: none"> <li>• <code>Valpha</code>: a list with the (generalized) correlation matrices (<code>Valpha</code>) of the nested variogram models structures along with the constants (<code>gcr.constant</code>) added to the respective semi-variance matrices.</li> <li>• <code>Valphaxi</code>: the (generalized) correlation matrix <math>\mathbf{V}_{\alpha,\xi} = \mathbf{\Gamma}_{\alpha,\xi}/(\sigma_n^2 + \sigma^2)</math> that includes the spatial nugget effect.</li> <li>• <code>Valphaxi.inverse</code>: the inverse of <math>\mathbf{V}_{\alpha,\xi}</math>.</li> <li>• <code>log.det.Valphaxi</code>: <math>\log(\det(\mathbf{V}_{\alpha,\xi}))</math>.</li> </ul>
zhat.objects	a list of matrices in (partly) <i>compressed form</i> with the following components: <ul style="list-style-type: none"> <li>• <code>Aalphaxi</code>: the matrix <math>(\mathbf{X}^T \mathbf{V}_{\alpha,\xi}^{-1} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{V}_{\alpha,\xi}^{-1}</math>.</li> <li>• <code>Palphaxi</code>: the matrix <math>\mathbf{I} - \mathbf{X} \mathbf{A}_{\alpha,\xi}</math>.</li> <li>• <code>Valphaxi.inverse.Palphaxi</code>: the matrix <math>\mathbf{V}_{\alpha,\xi}^{-1} \mathbf{P}_{\alpha,\xi}</math>.</li> </ul>
locations.object	a list with 3 components: <ul style="list-style-type: none"> <li>• <code>locations</code>: a formula indicating the coordinates of the measurement locations.</li> <li>• <code>coordinates</code>: a numeric matrix with the coordinates of the measurement locations.</li> <li>• <code>lag.vectors</code>: a numeric matrix with the lag vectors between any distinct pairs of measurement locations.</li> </ul>
initial.objects	a list with 3 components: <ul style="list-style-type: none"> <li>• <code>coefficients</code>: initial estimates of <math>\beta</math> computed either by <code>lmrob</code> or <code>rq</code>.</li> <li>• <code>bhat</code>: initial predictions of <math>\mathbf{B}</math>.</li> <li>• <code>variogram.object</code>: the initial values of the parameters of a possibly nested variograms model. This is a list with the same structure as described above for the component <code>variogram.object</code>.</li> </ul>
hessian.tfpa	a symmetric matrix with the Hessian (observed Fisher information) at the solution with respect to the transformed variogram and anisotropy parameters if the model was fitted non-robustly with the argument <code>hessian = TRUE</code> (see <a href="#">control.georob</a> ). Missing otherwise. This Hessian is used by <a href="#">summary.georob</a> to compute confidence intervals for the estimated parameters.
hessian.ntfpa	a symmetric matrix with the Hessian (observed Fisher information) at the solution with respect to the non-transformed variogram and anisotropy parameters if the model was fitted non-robustly with the argument <code>hessian = TRUE</code> (see <a href="#">control.georob</a> ). Missing otherwise.
control	a list with control parameters generated by <a href="#">control.georob</a> .

MD optionally a matrix of robust distances in the space spanned by  $X$  (see argument `compute.rd` of `lmrob.control` and `control.georob`).

`model`, `x`, `y` if requested the model frame, the model matrix and the response, respectively.

`na.action`, `offset`, `contrasts`, `xlevels`, `rank`, `df.residual`, `call`, `terms` further components of the fit as described for an object of class `lm`.

### Author(s)

Andreas Papritz <papritz@retired.ethz.ch>.

### See Also

[georobPackage](#) for a description of the model and a brief summary of the algorithms;

[georob](#) for (robust) fitting of spatial linear models;

[profilelogLik](#) for computing profiles of Gaussian likelihoods;

[plot.georob](#) for display of RE(ML) variogram estimates;

[control.georob](#) for controlling the behaviour of `georob`;

[georobModelBuilding](#) for stepwise building models of class `georob`;

[cv.georob](#) for assessing the goodness of a fit by `georob`;

[georobMethods](#) for further methods for the class `georob`;

[predict.georob](#) for computing robust Kriging predictions;

[lgnp](#) for unbiased back-transformation of Kriging prediction of log-transformed data;

[georobSimulation](#) for simulating realizations of a Gaussian process from model fitted by `georob`;

and finally

[sample.variogram](#) and [fit.variogram.model](#) for robust estimation and modelling of sample variograms.

### Description

This page documents the methods `coef`, `fixef`, `fixed.effects`, `model.frame`, `model.matrix`, `nobs`, `print`, `ranef`, `random.effects`, `resid`, `residuals`, `rstandard`, `summary` and `vcov` for the class `georob` which extract the respective components or summarize a `georob` object.



**Usage**

```
## S3 method for class 'georob'
coef(object, what = c("trend", "variogram"), ...)

## S3 method for class 'georob'
fixef(object, ...)

## S3 method for class 'georob'
fixed.effects(object, ...)

## S3 method for class 'georob'
model.frame(formula, ...)

## S3 method for class 'georob'
model.matrix(object, ...)

## S3 method for class 'georob'
nobs(object, ...)

## S3 method for class 'georob'
print(x, digits = max(3, getOption("digits") - 3), ...)

## S3 method for class 'georob'
ranef(object, standard = FALSE, ...)

## S3 method for class 'georob'
random.effects(object, standard = FALSE, ...)

## S3 method for class 'georob'
resid(object,
  type = c("working", "response", "deviance", "pearson", "partial"),
  terms = NULL,
  level = 1, ...)

## S3 method for class 'georob'
residuals(object,
  type = c("working", "response", "deviance", "pearson", "partial"),
  terms = NULL,
  level = 1, ...)

## S3 method for class 'georob'
rstandard(model, level = 1, ...)

## S3 method for class 'georob'
summary(object, correlation = FALSE, signif = 0.95, ...)

## S3 method for class 'georob'
vcov(object, ...)
```

## Arguments

object, model, x	an object of class <code>georob</code> , see <a href="#">georobObject</a> .
formula	a model <a href="#">formula</a> or <a href="#">terms</a> object or an object of class <code>georob</code> , see <a href="#">georobObject</a> .
correlation	a logical scalar controlling whether the correlation matrix of the estimated regression coefficients and of the fitted variogram parameters (only for non-robust fits) is computed (default <code>FALSE</code> ).
digits	a positive integer indicating the number of decimal digits to print.
level	an optional integer giving the level for extracting the residuals from object. <code>level = 0</code> extracts the regression residuals $\hat{B}(s) + \hat{\varepsilon}(s)$ and <code>level = 1</code> (default) only the estimated errors $\hat{\varepsilon}(s)$ .
signif	a numeric with the confidence level for computing confidence intervals for variogram parameters (default <code>0.95</code> ).
standard	a logical scalar controlling whether the spatial random effects $B$ should be standardized (default <code>FALSE</code> ).
type	a character keyword indicating the type of residuals to compute, see <a href="#">residuals.lm</a> . <code>type = "huber"</code> computes 'huberized' residuals $\hat{\sigma}/\gamma_1 \psi(\hat{\varepsilon}(s)/\hat{\sigma})$ .
terms	If <code>type = "terms"</code> , which terms (default is all terms).
what	If <code>what = "trend"</code> (default) the function <code>coef</code> extracts the coefficients of the trend model and for <code>what = "variogram"</code> the variogram parameters.
...	additional arguments passed to methods.

## Details

For robust REML fits deviance returns (possibly with a warning) the deviance of the Gaussian REML fit of the equivalent Gaussian spatial linear model with heteroscedastic nugget.

The methods `model.frame`, `model.matrix` and `nobs` extract the model frame, model matrix and the number of observations, see help pages of respective generic functions.

The methods `residuals` (and `resid`) extract either the estimated independent errors  $\hat{\varepsilon}(s)$  or the sum of the latter quantities and the spatial random effects  $\hat{B}(s)$ . `rstandard` does the same but standardizes the residuals to unit variance. `ranef` (`random.effects`) extracts the spatial random effects with the option to standardize them as well, and `fixef` (`fixed.effects`) extracts the fitted fixed-effects regression coefficients, which may of course also be obtained by `coef`.

For Gaussian REML the method `summary` computes confidence intervals of the estimated variogram and anisotropy parameters from the Hessian matrix of the (restricted) log-likelihood (= observed Fisher information), based on the asymptotic normal distribution of (RE)ML estimates. Note that the Hessian matrix with respect to the *transformed* variogram and anisotropy parameters is used for this. Hence the inverse Hessian matrix is the covariance matrix of the transformed parameters, confidence intervals are first computed for the transformed parameters and the limits of these intervals are transformed back to the original scale of the parameters. Optionally, `summary` reports the correlation matrix of the *transformed* parameters, also computed from the Hessian matrix.

Note that the methods `coef` and `summary` generate objects of class `coef.georob` and `summary.georob`, respectively, for which only `print` methods are available.

Besides, the default methods of the generic functions `confint`, `df.residual`, `fitted`, `formula`, `termplot` and `update` can be used for objects of class `georob`.

### Value

The methods `fixef.georob` and `fixed.effects.georob` return the numeric vector of estimated fixed-effects regression coefficients, and `vcov.georob` returns the covariance matrix of the estimated regression coefficients.

The method `coef.georob` returns an object of class `coef.georob` which is a numeric vector with estimated fixed-effects regression coefficients or variogram and anisotropy parameters. There is a `print` method for objects of class `coef.georob` which returns invisibly the object unchanged.

The methods `resid.georob`, `residuals.georob` and `rstandard.georob` return numeric vectors of (standardized) residuals, and `ranef.georob` and `random.effects.georob` the numeric vector of (standardized) spatial random effects, see *Details*.

The methods `model.frame.georob` and `model.matrix.georob` return a model frame and the fixed-effects model matrix, respectively, and `nobs.georob` returns the number of observations used to fit a spatial linear model.

The method `summary.georob` generates an object of class `summary.georob` which is a list with components extracted directly from object (`call`, `residuals`, `bhat`, `rweights`, `converged`, `convergence.code`, `iter`, `loglik`, `variogram.object`, `gradient`, `tuning.psi`, `df.residual`, `control`, `terms`) and complemented by the following components:

`scale` the square root of the estimated nugget effect  $\tau^2$ .

`coefficients` a 4-column matrix with estimated regression coefficients, their standard errors, *t*-statistics and corresponding (two-sided) *p*-values.

`correlation` an optional [compressed](#) lower-triangular matrix with the Pearson correlation coefficients of the estimated regression coefficients.

`param.aniso` either a vector (robust REML) or a 3-column matrix (Gaussian REML) with estimated variogram and anisotropy parameters, complemented for Gaussian REML with confidence limits, see *Details*.

`cor.tf.param` an optional [compressed](#) lower-triangular matrix with the Pearson correlation coefficients of estimated transformed variogram and anisotropy parameters, see *Details*.

`se.residuals` a vector with the standard errors of the estimated  $\varepsilon$ .

There is a `print` methods for class `summary.georob` which invisibly returns the object unchanged.

The method `print.georob` invisibly returns the object unchanged.

### Author(s)

Andreas Papritz <papritz@retired.ethz.ch>.

### See Also

[georobPackage](#) for a description of the model and a brief summary of the algorithms;

[georob](#) for (robust) fitting of spatial linear models;

[georobObject](#) for a description of the class `georob`;

[profilelogLik](#) for computing profiles of Gaussian likelihoods;  
[plot.georob](#) for display of RE(ML) variogram estimates;  
[control.georob](#) for controlling the behaviour of georob;  
[georobModelBuilding](#) for stepwise building models of class georob;  
[cv.georob](#) for assessing the goodness of a fit by georob;  
[predict.georob](#) for computing robust Kriging predictions;  
[lgnpp](#) for unbiased back-transformation of Kriging prediction of log-transformed data;  
[georobSimulation](#) for simulating realizations of a Gaussian process from model fitted by georob;  
 and finally  
[sample.variogram](#) and [fit.variogram.model](#) for robust estimation and modelling of sample variograms.

## Examples

```

data(meuse)

## Gaussian REML fit
r.logzn.reml <- georob(log(zinc) ~ sqrt(dist), data = meuse, locations = ~ x + y,
  variogram.model = "RMexp",
  param = c(variance = 0.15, nugget = 0.05, scale = 200),
  tuning.psi = 1000)
summary(r.logzn.reml, correlation = TRUE)

## robust REML fit
r.logzn.rob <- update(r.logzn.reml, tuning.psi = 1)

summary(r.logzn.rob, correlation = TRUE)

## residual diagnostics
old.par <- par(mfrow = c(2,3))

plot(fitted(r.logzn.reml), rstandard(r.logzn.reml))
abline(h = 0, lty = "dotted")
qqnorm(rstandard(r.logzn.reml))
abline(0, 1)
qqnorm(ranef(r.logzn.reml, standard = TRUE))
abline(0, 1)
plot(fitted(r.logzn.rob), rstandard(r.logzn.rob))
abline(h = 0, lty = "dotted")
qqnorm(rstandard(r.logzn.rob))
abline(0, 1)
qqnorm(ranef(r.logzn.rob, standard = TRUE))
abline(0, 1)

par(old.par)

```

---

georobSimulation      *Simulating Realizations of Gaussian Processes*

---

## Description

This page documents the function `condsim` that simulates (un)conditional realizations of Gaussian processes from the parameters of a spatial linear model estimated by the function `georob`.

## Usage

```
condsim(object, newdata, nsim, seed, type = c("response", "signal"),
        locations, trend.coef = NULL,
        variogram.model = NULL, param = NULL, aniso = NULL, variogram.object = NULL,
        control = control.condsim(), verbose = 0)
```

```
control.condsim(use.grid = FALSE, grid.refinement = 2.,
                condsim = TRUE, ce.method = c("standard", "approximate" ),
                ce.grid.expansion = 1., include.data.sites = FALSE,
                means = FALSE, trend.covariates = FALSE, covariances = FALSE,
                ncores = 1, mmax = 10000, pcmp = control.pcmp())
```

## Arguments

<code>object</code>	an object of class <code>georob</code> (mandatory argument), see <code>georobObject</code> .
<code>newdata</code>	a mandatory data frame, <code>SpatialPointsDataFrame</code> , <code>SpatialPixelsDataFrame</code> , <code>SpatialGridDataFrame</code> , <code>SpatialPoints</code> , <code>SpatialPixels</code> or <code>SpatialGrid</code> object, with the coordinates of points for which simulations are computed and in which to look for variables required for computing fitted values or Kriging predictions, see <code>predict.georob</code> .
<code>nsim</code>	a positive interger with the number of (conditional) realizations to compute (mandatory argument).
<code>seed</code>	an integer seed to initialize random number generation, see <code>set.seed</code> (mandatory argument).
<code>type</code>	a character keyword defining what target quantity should be simulated. Possible values are <ul style="list-style-type: none"> <li>• "signal": the "signal" <math>Z(\mathbf{s}) = \mathbf{x}(\mathbf{s})^T \boldsymbol{\beta} + B(\mathbf{s})</math> of the process,</li> <li>• "response": the observations <math>Y(\mathbf{s}) = Z(\mathbf{s}) + \varepsilon(\mathbf{s})</math>, (default),</li> </ul> see <code>georobPackage</code> for details on the model specification.
<code>locations</code>	an optional one-sided formula specifying what variables of <code>newdata</code> are the coordinates of the points for which simulations are computed (default <code>object[["locations.objects"]][["locations"]]</code> ).
<code>trend.coef</code>	an optional numeric vector with the coefficients of the trend model to be used for computing the (conditional) mean function of the random process see <i>Details</i> .

variogram.model	an optional character keyword defining the variogram model to be used for the simulations, see <a href="#">georob</a> and <i>Details</i> .
param	an optional named numeric vector with values of the variogram parameters used for the simulations, see <a href="#">georob</a> and <i>Details</i> .
aniso	an optional named numeric vector with values of anisotropy parameters of a variogram used for the simulations, see <a href="#">georob</a> and <i>Details</i> .
variogram.object	an optional list that defines a possibly nested variogram model used for the simulations, see <a href="#">georob</a> and <i>Details</i> .
control	a list with the components <code>use.grid</code> , <code>grid.refinement</code> , <code>condsim</code> , <code>ce.method</code> , <code>ce.grid.expansion</code> , <code>include.data.sites</code> , <code>means</code> , <code>trend.covariates</code> , <code>covariances</code> , <code>ncores</code> , <code>mmax</code> and <code>pcmp</code> or a function such as <code>control.condsim</code> that generates such a list, see arguments of <code>control.condsim</code> for details.
verbose	a positive integer controlling logging of diagnostic messages to the console. <code>verbose = 0</code> (default) suppresses such messages.
use.grid	a logical scalar (default FALSE) to control whether (conditional) realizations are computed for a rectangular grid instead of the coordinates of points contained in <code>newdata</code> , see <i>Details</i> .
grid.refinement	a numeric that defines a factor by which the minimum differences of the coordinates between any pair of points in <code>newdata</code> are divided to setup the simulation grid, should be $> 1$ (default 2), see <i>Details</i> .
condsim	a logical scalar to control whether conditional (TRUE default) or unconditional simulations (FALSE) are computed.
ce.method	a character keyword to select the method to simulate realizations by the circulant embedding algorithm, see <i>Details</i> .
ce.grid.expansion	a numeric with the factor by which the dimensions of the simulation grid is expanded in the circulant embedding algorithm. Should be $\geq 1$ (default 1).
include.data.sites	a logical scalar, to control whether (conditionally) simulated values are computed also for the points of the original data set used to estimate the model parameters and contained in <code>object</code> .
means	a logical scalar, to control whether the (un)conditional means are included in the output.
trend.covariates	a logical scalar, to control whether the covariates required for the trend model are included in the output.
covariances	a logical scalar, to control whether the covariances between the points of the original data set used to estimate the model parameters ( <code>attr gcvmat.d.d</code> , <a href="#">compressed matrix</a> ) and the covariances between the simulation and the original data points ( <code>attr gcvmat.s.d</code> , <code>matrix</code> ) are returned as attributes of the output. Note that these covariances are only returned if <code>condsim = TRUE</code> .

ncores	a positive integer controlling how many cores are used for parallelized computations, defaults to 1.
mmax	a positive integer equal to the maximum number (default 10000) of prediction items, computed in sub-tasks executed in parallel, see section <i>Details of predict.georob</i> .
pcmp	a list of arguments, passed e.g. to <code>pmm</code> or a function such as <code>control.pcmp</code> that generates such a list (see <code>control.pcmp</code> for allowed arguments).

## Details

### General:

`condsim` (conditionally) simulates from a Gaussian process that has a linear mean function with parameters  $\beta$  and an auto-correlation structure characterized by a parametric variogram model and variogram parameters  $\tau^2$  and  $\theta$  (see `georobPackage` for the employed parametrization of the spatial linear model). The parameters of the mean and auto-correlation function are either taken from the spatial linear model estimated by `georob` and passed by the argument `object` to `condsim` or from the optional arguments `trend.coef` ( $\beta$ ) and `variogram.model`, `param`, `aniso` or `variogram.object` ( $\tau^2$ ,  $\theta$ ).

Simulated values are computed for the points in `newdata` and optionally also for the data points in `object` if `include.data.sites = TRUE`. Both unconditional and conditional simulations can be computed. In the latter cases, the simulated values are always conditioned to the response data used to fit the spatial linear model by `georob` and contained in `object`.

### Unconditional simulation:

Unconditional realizations are either computed for the exact locations of the points in `newdata` (`use.grid = FALSE`), irrespective of the fact whether these are arranged on a regular grid or not. Simulations are then generated by the Cholesky matrix decomposition method (e.g. *Chilès and Delfiner, 1999, sec. 7.2.2*).

For `use.grid = TRUE` the points in `newdata` are matched to a rectangular simulation grid and the simulations are generated for all nodes of this grid by the circulant embedding method (*Davis and Bryant, 2013; Dietrich and Newsam, 1993; Wood and Chan, 1994*). For large problems this approach may be substantially faster and less memory demanding than the Cholesky matrix decomposition method.

For circulant embedding, first a rectangular simulation grid is constructed from the coordinates of the points in `newdata` and `object`. The spacings of the simulation grid is equal to the minimum coordinate differences between any pair of points in `newdata`, divided by `grid.refinement`. The spatial extent of the simulation grid is chosen such that it covers the bounding boxes of all points in `newdata` and `object`. The points in `newdata` and `object` are then matched to the closest nodes of the simulation grid. If the same node is assigned to a point in `object` and `newdata` then the point in `object` is kept and the concerned point in `newdata` is omitted.

The rectangular simulation grid is then expanded to the larger circulant embedding grid, and the eigenvalues of the so-called *base matrix* (= first row of the covariance matrix of the nodes of the circulant embedding grid with block circulant structure, see *Davies and Bryant, 2013*) are computed by fast discrete Fourier transform (FFT). It may happen that some of the eigenvalues of the base matrix are negative. The standard circulant embedding algorithm then fails.

Two approaches are implemented in `condsim` to handle this situation:

- First, one may use the *approximate circulant embedding* method by choosing `ce.method = "approximate"`. This sets the negative eigenvalues of the base matrix to zero and scales the eigenvalues, see *Chan and Wood (1994, sec. 4, choice  $\rho = \rho_2$ )*.
- Second, one may attempt to avoid the problem of negative eigenvalues by increasing the size of the simulation (and circulant embedding) grids. This can be achieved by choosing a value  $> 1$  for the argument `ce.grid.expansion`, see respective parts in *Dietrich and Newsam (1993, sec. 4)* and *Wood and Chan (1994, sec. 3)*.

Note that the dimension of the simulation and embedding grids are chosen such that the number of nodes is a highly composite integer. This allows efficient FFT.

#### Conditional simulation:

For both the Cholesky matrix decomposition and the circulant embedding approach, simulations are conditioned to data by the Kriging method, see *Chilès and Delfiner, 1999, sec. 7.3*.

#### Parallelized computations:

`condsim` uses the packages **parallel** and **snowfall** for parallelized computations. Three tasks can be executed in parallel:

- Computation of (generalized correlations), see `control.pcmp` how to do this.
- Computation of Kriging predictions required for conditional simulations, see section *Details* of `predict.georob`.
- Fast Fourier transform of realizations of standard normal deviates generated for the nodes of the base matrix (see *Davies and Bryant, 2013, steps 3–5 of algorithm*). If there are `nsim` realizations to simulate, the task is split into `ceiling(nsim / ncores)` sub-tasks that are then distributed to `ncores` CPUs. Evidently, `ncores = 1` (default) suppresses parallel execution.

#### Value

The output generated by `condsim` is an object of a “similar” class as `newdata` (data frame, `SpatialPointsDataFrame`, `SpatialPixelsDataFrame`, `SpatialGridDataFrame`, `SpatialPolygonsDataFrame`).

The data frame or the data slot of the `Spatial...DataFrame` objects have the following components:

- the coordinates of the prediction points (only present if `newdata` is a data frame).
- `expct`: optionally the (un)conditional means.
- optionally the covariates required for the trend model.
- `sim.1, sim.2, ...`: the (un)conditionally simulated realizations.

The function `control.condsim` returns a list with parameters to steer `condsim`, see arguments above.

#### Author(s)

Andreas Papritz <papritz@retired.ethz.ch>.



## References

- Chilès, J.-P., Delfiner, P. (1999) *Geostatistics Modeling Spatial Uncertainty*, Wiley, New York, doi:10.1002/9780470316993.
- Davies, T. M., Bryant, D. (2013) On circulant embedding for gaussian random fields in R, *Journal of Statistical Software*, **55**, 1–21, doi:10.18637/jss.v055.i09.
- Dietrich, C. R., Newsam, G. N. (1993) A fast and exact method for multidimensional gaussian stochastic simulations, *Water Resources Research*, **9**, 2861–2869, doi:10.1029/93WR01070.
- Wood, A. T. A., Chan, G. (1994) Simulation of stationary gaussian processes in  $[0, 1]^d$ , *Journal of Computational and Graphical Statistics*, **3**, 409–432, doi:10.2307/1390903.

## See Also

[georobPackage](#) for a description of the model and a brief summary of the algorithms;

[georob](#) for (robust) fitting of spatial linear models;

[georobObject](#) for a description of the class georob;

[profilelogLik](#) for computing profiles of Gaussian likelihoods;

[plot.georob](#) for display of RE(ML) variogram estimates;

[control.georob](#) for controlling the behaviour of georob;

[georobModelBuilding](#) for stepwise building models of class georob;

[cv.georob](#) for assessing the goodness of a fit by georob;

[georobMethods](#) for further methods for the class georob;

[predict.georob](#) for computing robust Kriging predictions;

[lgnpp](#) for unbiased back-transformation of Kriging prediction of log-transformed data;

[sample.variogram](#) and [fit.variogram.model](#) for robust estimation and modelling of sample variograms.

## Examples

```
data(meuse)
data(meuse.grid)

## convert to SpatialGridDataFrame
meuse.grid.sgdf <- meuse.grid
coordinates(meuse.grid.sgdf) <- ~ x + y
gridded(meuse.grid.sgdf) <- TRUE
fullgrid(meuse.grid.sgdf) <- TRUE

## Gaussian REML fit
r.logzn.reml <- georob(log(zinc) ~ sqrt(dist), data = meuse,
  locations = ~ x + y, variogram.model = "RMexp",
  param = c(variance = 0.15, nugget = 0.05, scale = 200),
  tuning.psi = 1000)

## Unconditional simulations using circulant embedding on rectangular
## simulation grid
```

```

r.sim.1 <- condsim(r.logzn.reml, newdata = meuse.grid.sgdf, nsim = 2, seed = 1,
  control = control.condsim(use.grid = TRUE, condsim = FALSE))
spplot(r.sim.1, zcol = "sim.1", at = seq(3.5, 8.5, by = 0.5))

## Conditional simulations using circulant embedding
if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s
  r.sim.2 <- condsim(r.logzn.reml, newdata = meuse.grid.sgdf, nsim = 2, seed = 1,
    control = control.condsim(use.grid = FALSE, condsim = TRUE))
  spplot(r.sim.2, zcol = "sim.2", at = seq(3.5, 8.5, by = 0.5))
}

```

## Description

The function `lgnpp` back-transforms point or block Kriging predictions of a log-transformed response variable computed by `predict.georob`. Alternatively, the function averages log-normal point Kriging predictions for a block and approximates the mean squared prediction error of the block mean.

## Usage

```
lgnpp(object, newdata, locations, is.block = FALSE, all.pred = NULL,
  extended.output = FALSE)
```

## Arguments

<code>object</code>	an object with Kriging predictions of a log-transformed response variable as obtained by <code>predict(georob-object, ...)</code> .
<code>newdata</code>	an optional object as passed as argument <code>newdata</code> to <code>predict.georob</code> , see <i>Details</i> .
<code>locations</code>	an optional one-sided formula specifying what variables of <code>newdata</code> are the coordinates of the prediction points, see <code>predict.georob</code> .
<code>is.block</code>	an optional logical scalar (default <code>FALSE</code> ) specifying whether point predictions contained in <code>object</code> are considered to belong to a single block and should be averaged after back-transformation. Ignored if <code>object</code> contains block Kriging predictions, see <i>Details</i> .
<code>all.pred</code>	an optional positive integer or an object as obtained by <code>lgnpp(predict(georob-object, ...))</code> , see <i>Details</i> .
<code>extended.output</code>	a logical scalar controlling whether the covariance matrix of the errors of the back-transformed point predictions is added as an attribute to the result, see <i>Details</i> .

## Details

The function `lgnpp` performs three tasks:

### 1. Back-transformation of point Kriging predictions of a log-transformed response:

The usual, marginally unbiased back-transformation for log-normal point Kriging is used:

$$\widehat{U}(\mathbf{s}) = \exp(\widehat{Z}(\mathbf{s}) + 1/2(\text{Var}_{\hat{\theta}}[Z(\mathbf{s})] - \text{Var}_{\hat{\theta}}[\widehat{Z}(\mathbf{s})])),$$

$$\begin{aligned} \text{Cov}_{\hat{\theta}}[U(\mathbf{s}_i) - \widehat{U}(\mathbf{s}_i), U(\mathbf{s}_j) - \widehat{U}(\mathbf{s}_j)] &= \mu_{\hat{\theta}}(\mathbf{s}_i)\mu_{\hat{\theta}}(\mathbf{s}_j) \\ &\times \{\exp(\text{Cov}_{\hat{\theta}}[Z(\mathbf{s}_i), Z(\mathbf{s}_j)]) - 2 \exp(\text{Cov}_{\hat{\theta}}[\widehat{Z}(\mathbf{s}_i), Z(\mathbf{s}_j)]) + \exp(\text{Cov}_{\hat{\theta}}[\widehat{Z}(\mathbf{s}_i), \widehat{Z}(\mathbf{s}_j)])\}, \end{aligned}$$

where  $\widehat{Z}$  and  $\widehat{U}$  denote the log- and back-transformed predictions of the signal, and

$$\mu_{\hat{\theta}}(\mathbf{s}) \approx \exp(\mathbf{x}(\mathbf{s})^T \widehat{\boldsymbol{\beta}} + 1/2 \text{Var}_{\hat{\theta}}[Z(\mathbf{s})]).$$

The expressions for the required covariance terms can be found in the Appendices of *Nussbaum et al. (2014)*. Instead of the signal  $Z(\mathbf{s})$ , predictions of the log-transformed response  $Y(\mathbf{s})$  or the estimated trend  $\mathbf{x}(\mathbf{s})^T \widehat{\boldsymbol{\beta}}$  of the log-transformed data can be back-transformed (see [georobPackage](#)). The above transformations are used if object contains point Kriging predictions (see `predict.georob`, *Value*) and if `is.block = FALSE` and `all.pred` is missing.

### 2. Back-transformation of block Kriging predictions of a log-transformed response:

Block Kriging predictions of a log-transformed response variable are back-transformed by the approximately unbiased transformation proposed by *Cressie (2006, Appendix C)*

$$\widehat{U}(A) = \exp(\widehat{Z}(A) + 1/2\{\text{Var}_{\hat{\theta}}[Z(\mathbf{s})] + \widehat{\boldsymbol{\beta}}^T \mathbf{M}(A) \widehat{\boldsymbol{\beta}} - \text{Var}_{\hat{\theta}}[\widehat{Z}(A)]\}),$$

$$E_{\hat{\theta}}[\{U(A) - \widehat{U}(A)\}^2] = \mu_{\hat{\theta}}(A)^2 \{\exp(\text{Var}_{\hat{\theta}}[Z(A)]) - 2 \exp(\text{Cov}_{\hat{\theta}}[\widehat{Z}(A), Z(A)]) + \exp(\text{Var}_{\hat{\theta}}[\widehat{Z}(A)])\}$$

where  $\widehat{Z}(A)$  and  $\widehat{U}(A)$  are the log- and back-transformed predictions of the block mean  $U(A)$ , respectively,  $\mathbf{M}(A)$  is the spatial covariance matrix of the covariates

$$\mathbf{M}(A) = 1/|A| \int_A (\mathbf{x}(\mathbf{s}) - \mathbf{x}(A))(\mathbf{x}(\mathbf{s}) - \mathbf{x}(A))^T d\mathbf{s}$$

within the block  $A$  where

$$\mathbf{x}(A) = 1/|A| \int_A \mathbf{x}(\mathbf{s}) d\mathbf{s}$$

and

$$\mu_{\hat{\theta}}(A) \approx \exp(\mathbf{x}(A)^T \widehat{\boldsymbol{\beta}} + 1/2 \text{Var}_{\hat{\theta}}[Z(A)]).$$

This back-transformation is based on the assumption that both the point data  $U(\mathbf{s})$  and the block means  $U(A)$  follow log-normal laws, which strictly cannot hold. But for small blocks the assumption works well as the bias and the loss of efficiency caused by this assumption are small (*Cressie, 2006; Hofer et al., 2013*).

The above formulae are used by `lgnpp` if object contains block Kriging predictions in the form of a `SpatialPolygonsDataFrame`. To approximate  $M(A)$ , one needs the covariates on a fine grid for the whole study domain in which the blocks lie. The covariates are passed `lgnpp` as argument `newdata`, where `newdata` can be any spatial data frame accepted by `predict.georob`. For evaluating  $M(A)$  the geometry of the blocks is taken from the polygons slot of the `SpatialPolygonsDataFrame` passed as object to `lgnpp`.

### 3. Back-transformation and averaging of point Kriging predictions of a log-transformed response:

`lgnpp` allows as a further option to back-transform and *average* point Kriging predictions passed as object to the function. One then assumes that the predictions in object refer to points that lie in a *single* block. Hence, one uses the approximation

$$\widehat{U}(A) \approx \frac{1}{K} \sum_{s_i \in A} \widehat{U}(s_i)$$

to predict the block mean  $U(A)$ , where  $K$  is the number of points in  $A$ . The mean squared prediction error can be approximated by

$$E_{\hat{\theta}}[\{U(A) - \widehat{U}(A)\}^2] \approx \frac{1}{K^2} \sum_{s_i \in A} \sum_{s_j \in A} \text{Cov}_{\hat{\theta}}[U(s_i) - \widehat{U}(s_i), U(s_j) - \widehat{U}(s_j)].$$

In most instances, the evaluation of the above double sum is not feasible because a large number of points is used to discretize the block  $A$ . `lgnpp` then uses the following approximations to compute the mean squared error (see also Appendix E of *Nussbaum et al., 2014*):

- Point prediction results are passed as object to `lgnpp` only for a *random sample of points in*  $A$  (of size  $k$ ), for which the evaluation of the above double sum is feasible.
- The prediction results for the *complete set of points* within the block are passed as argument `all.pred` to `lgnpp`. These results are used to compute  $\widehat{U}(A)$ .
- The mean squared error is then approximated by

$$E_{\hat{\theta}}[\{U(A) - \widehat{U}(A)\}^2] \approx \frac{1}{K^2} \sum_{s_i \in A} E_{\hat{\theta}}[\{U(s_i) - \widehat{U}(s_i)\}^2] \\ + \frac{K-1}{Kk(k-1)} \sum_{s_i \in \text{sample}} \sum_{s_j \in \text{sample}, s_j \neq s_i} \text{Cov}_{\hat{\theta}}[U(s_i) - \widehat{U}(s_i), U(s_j) - \widehat{U}(s_j)].$$

The first term of the RHS (and  $\widehat{U}(A)$ ) can be computed from the point Kriging results contained in `all.pred`, and the double sum is evaluated from the full covariance matrices of the predictions and the respective targets, passed to `lgnpp` as object (one has to use the arguments `control=control.predict.georob(full.covmat=TRUE)` for `predict.georob` when computing the point Kriging predictions stored in object).

- If the prediction results are not available for the complete set of points in  $A$  then `all.pred` may be equal to  $K$ . The block mean is then approximated by

$$\widehat{U}(A) \approx \frac{1}{k} \sum_{s_i \in \text{sample}} \widehat{U}(s_i)$$

and the first term of the RHS of the expression for the mean squared error by

$$\frac{1}{kK} \sum_{s_i \in \text{sample}} E_{\hat{\theta}}[\{U(s_i) - \hat{U}(s_i)\}^2].$$

- By drawing samples repeatedly and passing the related Kriging results as object to `lgnpp`, one can reduce the error of the approximation of the mean squared error.

### Value

If `is.block` is FALSE and `all.pred` is equal to NULL `lgnpp` returns an updated object of the same class as object (see section *Value* of `predict.georob`). The data frame with the point or block Kriging predictions is complemented by `lgnpp` with the following new components:

- `lgn.pred`: the back-transformed Kriging predictions of a log-transformed response.
- `lgn.se`: the standard errors of the back-transformed predictions.
- `lgn.lower`, `lgn.upper`: the bounds of the back-transformed prediction intervals.

If `is.block` is TRUE or `all.pred` not equal to NULL `lgnpp` returns a named numeric vector with two elements:

- `mean`: the back-transformed block Kriging estimate, see *Details*.
- `se`: the (approximated) block Kriging standard error, see *Details*.

If `extended.output` is TRUE then the vector is supplemented with the attribute `mse.lgn.pred` that contains the full covariance matrix of the back-transformed point prediction errors.

### Author(s)

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### References

- Cressie, N. (2006) Block Kriging for Lognormal Spatial Processes. *Mathematical Geology*, **38**, 413–443, doi:10.1007/s1100400590228.
- Hofer, C., Borer, F., Bono, R., Kayser, A. and Papritz, A. 2013. Predicting topsoil heavy metal content of parcels of land: An empirical validation of customary and constrained lognormal block Kriging and conditional simulations. *Geoderma*, **193–194**, 200–212, doi:10.1016/j.geoderma.2012.08.034.
- Nussbaum, M., Papritz, A., Baltensweiler, A. and Walthert, L. (2014) Estimating soil organic carbon stocks of Swiss forest soils by robust external-drift kriging. *Geoscientific Model Development*, **7**, 1197–1210. doi:10.5194/gmd711972014.

### See Also

`georobPackage` for a description of the model and a brief summary of the algorithms;  
`georob` for (robust) fitting of spatial linear models;  
`predict.georob` for computing robust Kriging predictions.

**Examples**

```

data(meuse)

data(meuse.grid)
coordinates(meuse.grid) <- ~x+y
meuse.grid.pixdf <- meuse.grid
gridded(meuse.grid.pixdf) <- TRUE

data(meuse.blocks, package = "constrainedKriging")

r.logzn.rob <- georob(log(zinc) ~ sqrt(dist), data = meuse, locations = ~ x + y,
  variogram.model = "RMexp", param = c(variance = 0.15, nugget = 0.05, scale = 200),
  tuning.psi = 1., control = control.georob(cov.bhat = TRUE, full.cov.bhat = TRUE))

## point predictions of log(Zn)
r.pred.points.1 <- predict(r.logzn.rob, newdata = meuse.grid.pixdf,
  control = control.predict.georob(extended.output = TRUE))
str(r.pred.points.1, max = 3)

## back-transformation of point predictions
r.backtf.pred.points <- lgnpp(r.pred.points.1)
str(r.backtf.pred.points, max = 3)

spplot(r.backtf.pred.points, zcol = "lgn.pred", main = "Zn content")

## predicting mean Zn content for whole area
if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s
  ## recompute point predictions with argument full.covmat = TRUE
  r.pred.points.2 <- predict(r.logzn.rob, newdata = meuse.grid.pixdf,
    control = control.predict.georob(extended.output = TRUE, full.covmat = TRUE))
  str(r.pred.points.2, max = 3)
  r.block <- lgnpp(r.pred.points.2, is.block = TRUE, all.pred = r.backtf.pred.points@data)
  r.block
}

## block predictions of log(Zn)
if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s
  r.pred.block <- predict(r.logzn.rob, newdata = meuse.blocks,
    control = control.predict.georob(extended.output = TRUE,
      pwidth = 75, pheight = 75, mmax = 50))
  r.backtf.pred.block <- lgnpp(r.pred.block, newdata = meuse.grid)

  spplot(r.backtf.pred.block, zcol = "lgn.pred", main = "block means Zn content")
}

```

**Description**

Auxiliary functions to query names and permissible ranges of variogram parameters.

**Usage**

```
param.names(model)
param.bounds(model, d)
```

**Arguments**

`model` a character keyword denoting a valid variogram, see [georob](#) and [georobPackage](#).  
`d` a positive integer with the number of dimensions of the survey domain.

**Value**

Either a character vector with the names of the additional variogram parameters such as the smoothness parameter of the Whittle-Matérn model (`param.names`) or a named list with the lower and upper bounds of permissible parameter ranges.

**Author(s)**

Andreas Papritz <papritz@retired.ethz.ch>.

**See Also**

[georobPackage](#) for a description of the model and a brief summary of the algorithms;  
[georob](#) for (robust) fitting of spatial linear models.

**Examples**

```
param.names("RMgengneiting")
param.bounds("RMgengneiting", d = 2)
```

---

plot.georob

*Plot Methods for Class georob*

---

**Description**

The `plot` and `lines` methods for class `georob` plot the variogram model, estimated by (robust) restricted maximum likelihood. `plot.georob` computes and plots in addition the sample variogram of the (robust) regression residuals and can be used to generate residual diagnostics plots (Tukey-Anscombe plot, normal QQ plots of residuals and random effects).

**Usage**

```
## S3 method for class 'georob'
plot(x, what = c("variogram", "covariance", "correlation",
  "ta", "sl", "qq.res", "qq.ranef" ), add = FALSE, lag.dist.def,
  xy.angle.def = c(0, 180), xz.angle.def = c(0, 180), max.lag = Inf,
  estimator = c("mad", "qn", "ch", "matheron"), mean.angle = TRUE,
  level = what != "ta", smooth = what == "ta" || what == "sl",
  id.n = 3, labels.id = names(residuals(x)), cex.id = 0.75,
  label.pos = c(4,2), col, pch, xlab, ylab, main, lty = "solid", ...)

## S3 method for class 'georob'
lines(x, what = c("variogram", "covariance", "correlation"),
  from = 1.e-6, to, n = 501, xy.angle = 90, xz.angle = 90,
  col = 1:length(xy.angle), pch = 1:length(xz.angle), lty = "solid", ...)
```

**Arguments**

x	an object of class <code>georob</code> , see <a href="#">georobObject</a> .
what	a character keyword for the quantity that should be displayed. Possible values are: <ul style="list-style-type: none"> <li>• "variogram": the variogram</li> <li>• "covariance": the covariance function</li> <li>• "correlation": the correlation function</li> <li>• "scale-location": square root of absolute regression residuals plotted against fitted values (Scale-Location plot)</li> <li>• "ta": regression residuals plotted against fitted values (Tukey-Anscombe plot)</li> <li>• "qq.res": normal Q-Q plot of standardized errors <math>\hat{\varepsilon}</math></li> <li>• "qq.ranef": normal Q-Q plot of standardized random effects <math>\hat{B}</math></li> </ul>
add	a logical scalar controlling whether a new plot should be generated (FALSE, default) or whether the information should be added to the current plot (TRUE).
lag.dist.def	an optional numeric scalar defining a constant bin width for grouping the lag distances or an optional numeric vector with the upper bounds of a set of contiguous bins for computing the sample variogram of the regression residuals, see <a href="#">sample.variogram</a> . If missing then the sample variogram is not computed.
xy.angle.def	an numeric vector defining angular classes in the horizontal plane for computing directional variograms. <code>xy.angle.def</code> must contain an ascending sequence of azimuth angles in degrees from north (positive clockwise to south), see <a href="#">sample.variogram</a> . Omnidirectional variograms are computed with the default <code>c(0, 180)</code> .
xz.angle.def	an numeric vector defining angular classes in the $x$ - $z$ -plane for computing directional variograms. <code>xz.angle.def</code> must contain an ascending sequence of angles in degrees from zenith (positive clockwise to nadir), see <a href="#">sample.variogram</a> . Omnidirectional variograms are computed with the default <code>c(0, 180)</code> .
max.lag	a positive numeric defining the largest lag distance for which semi-variances should be computed (default no restriction).



estimator	a character keyword defining the estimator for computing the sample variogram. Possible values are: <ul style="list-style-type: none"> <li>• "qn": Genton's robust <math>Q_n</math>-estimator (default, <i>Genton, 1998</i>),</li> <li>• "mad": Dowd's robust MAD-estimator (<i>Dowd, 1984</i>),</li> <li>• "matheron": non-robust method-of-moments estimator,</li> <li>• "ch": robust Cressie-Hawkins estimator (<i>Cressie and Hawkins, 1980</i>).</li> </ul>
mean.angle	a logical scalar controlling whether the mean lag vector (per combination of lag distance and angular class) is computed from the mean angles of all the lag vectors falling into a given class (TRUE, default) or from the mid-angles of the respective angular classes (FALSE).
level	an integer giving the level for extracting the residuals from object for what = "ta" or what = "qq.res". level = 0 (default for what == "ta") extracts the regression residuals $\hat{B}(s) + \hat{\varepsilon}(s)$ and level = 1 (default for what == "qq.res") only the estimated errors $\hat{\varepsilon}(s)$ .
smooth	a logical scalar controlling whether a <code>loess.smooth</code> is added to the Tukey-Anscombe plot (default TRUE).
id.n	a numeric with the number of points to be labelled in each plot, starting with the most extreme (see <code>plot.lmrob</code> ).
labels.id	a vector of labels, from which the labels for extreme points will be chosen (see <code>plot.lmrob</code> ). NULL uses observation numbers.
cex.id	a numeric with the magnification of point labels (see <code>plot.lmrob</code> ).
label.pos	a numeric for positioning of labels, for the left half and right half of the graph respectively (see <code>plot.lmrob</code> ).
from	a numeric with the minimal lag distance for plotting variogram models.
to	a numeric with the maximum lag distance for plotting variogram models (default: largest lag distance of current plot).
n	a positive integer specifying the number of equally spaced lag distances for which semi-variances are evaluated in plotting variogram models (default 501).
xy.angle	a numeric (vector) with azimuth angles (in degrees, clockwise positive from north) in $x$ - $y$ -plane for which semi-variances should be plotted.
xz.angle	a numeric (vector) with angles in $x$ - $z$ -plane (in degrees, clockwise positive from zenith to south) for which semi-variances should be plotted.
col	an optional vector with colours of points and curves to distinguish items relating to different azimuth angles in $x$ - $y$ -plane.
pch	an optional vector with symbols for points and curves to distinguish items relating to different azimuth angles in $x$ - $z$ -plane.
lty	line type for plotting variogram models.
xlab, ylab, main	plot annotation, see <code>plot</code> .
...	additional arguments passed to <code>plot.sample.variogram</code> , <code>loess.smooth</code> and graphical methods.

**Value**

The method `plot.georob` returns no value, it is called for its side effects.

The method `lines.georob` is called for its side effects and returns the value `NULL` invisibly.

**Author(s)**

Andreas Papritz <papritz@retired.ethz.ch>.

**See Also**

[georobPackage](#) for a description of the model and a brief summary of the algorithms;

[georob](#) for (robust) fitting of spatial linear models;

[georobObject](#) for a description of the class `georob`;

[profilelogLik](#) for computing profiles of Gaussian likelihoods;

[control.georob](#) for controlling the behaviour of `georob`;

[georobModelBuilding](#) for stepwise building models of class `georob`;

[cv.georob](#) for assessing the goodness of a fit by `georob`;

[georobMethods](#) for further methods for the class `georob`;

[predict.georob](#) for computing robust Kriging predictions;

[lgnpp](#) for unbiased back-transformation of Kriging prediction of log-transformed data;

[georobSimulation](#) for simulating realizations of a Gaussian process from model fitted by `georob`;  
and finally

[sample.variogram](#) and [fit.variogram.model](#) for robust estimation and modelling of sample variograms.

**Examples**

```
#####
## meuse data ##
#####
data(meuse)

## Gaussian REML fit
r.logzn.reml <- georob(log(zinc) ~ sqrt(dist), data = meuse, locations = ~ x + y,
  variogram.model = "RMexp",
  param = c(variance = 0.15, nugget = 0.05, scale = 200),
  tuning.psi = 1000)
summary(r.logzn.reml, correlation = TRUE)
plot(r.logzn.reml, lag.dist.def = seq(0, 2000, by = 100))

## robust REML fit
if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s
  r.logzn.rob <- update(r.logzn.reml, tuning.psi = 1)

  summary(r.logzn.rob, correlation = TRUE)
```

```

    lines(r.logzn.rob, col = "red")
}

```

pmm

*Parallelized Matrix Multiplication***Description**

This page documents the function `pmm` for parallelized matrix multiplication and the function `control.pcmp`, which controls the behaviour of `pmm` and other functions that execute tasks in parallel.

**Usage**

```
pmm(A, B, control = control.pcmp())
```

```
control.pcmp(pmm.ncores = 1, gcr.ncores = 1, max.ncores = parallel::detectCores(),
  f = 1, sfstop = FALSE, allow.recursive = FALSE,
  fork = !identical(.Platform[["OS.type"]], "windows"), ...)
```

**Arguments**

A, B	two numeric matrices to be multiplied.
control	a list with the arguments <code>pmm.ncores</code> , <code>gcr.ncores</code> , <code>max.ncores</code> , <code>f</code> , <code>sfstop</code> and <code>allow.recursive</code> or a function such as <code>control.pcmp</code> that generates such a list.
pmm.ncores	an integer (default 1) with the number of cores used for parallelized matrix multiplication.
gcr.ncores	an integer (default 1) with the number of cores used for parallelized computation of (generalized) covariances or semi-variances.
max.ncores	maximum number of cores (integer, default all cores of a machine) used for parallelized computations.
f	an integer (default 1) with the number of tasks assigned to each core in parallelized operations.
sfstop	a logical scalar controlling whether the SNOW socket cluster is stopped after each parallelized matrix multiplication on windows OS (default FALSE).
allow.recursive	a logical scalar controlling whether parallelized matrix multiplication and computation of (generalized) covariances should be allowed by child processes running already in parallel (default FALSE).
fork	a logical scalar controlling whether forking should be used for parallel computations (default TRUE on unix and FALSE on windows operating systems). Note that setting <code>fork = TRUE</code> on windows suppresses parallel computations.
...	further arguments, currently not used.

## Details

Parallelized matrix multiplication shortens computing time for large data sets ( $n > 1000$ ). However, spawning child processes requires itself resources and increasing the number of cores for parallelized matrix multiplication and parallelized computation of covariances does not always result in reduced computing time. Furthermore, these operations may be initiated by child processes, that were itself spawned by functions like `cv.georob`, `predict.georob`, `profilelogLik`, `add1.georob`, `drop1.georob` and `step.georob`. By default, parallelized matrix multiplication and computation of covariances is then suppressed to avoid that child processes itself spawn child processes. To allow parallelized matrix multiplication and parallelized computation of covariances by child processes one has to use the argument `allow.recursive = TRUE`.

Note that very substantial reductions in computing time results when one uses the **OpenBLAS** library instead of the reference BLAS library that ships with R, see <https://www.openblas.net/> and R FAQ for your OS. With OpenBLAS no gains are obtained by using more than one core for matrix multiplication, and one should therefore use the default arguments `pmm.ncores = 1` for `control.pcmp()`.

`max.ncores` controls how many child processes are spawned in total. This can be used to prevent that child processes spawn themselves children which may result in a considerable number of child processes.

## Value

`pmm`: the matrix product `A %*% B`,

`control.pcmp`: a list with components `pmm.ncores`, `gcr.ncores`, `max.ncores`, `f`, `sfstop`, `allow.recursive`.

## Author(s)

Andreas Papritz <papritz@retired.ethz.ch>.

## See Also

[georobPackage](#) for a description of the model and a brief summary of the algorithms;

[georob](#) for (robust) fitting of spatial linear models.

## Examples

```
if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s
  A <- as.matrix(dist(rnorm(2000)))
  B <- as.matrix(dist(rnorm(2000)))
  system.time(C <- A %*% B)
  system.time(C <- pmm(
    A, B, control = control.pcmp(pmm.ncores = 2L)))
}
```

---

predict.georob                      *Predict Method for Robustly Fitted Spatial Linear Models*

---

## Description

Robust and customary external drift Kriging prediction based on a spatial linear models fitted by georob. The predict method for the class georob computes fitted values, point and block Kriging predictions as well as model terms for display by [termplot](#).

## Usage

```
## S3 method for class 'georob'
predict(object, newdata, type = c("signal", "response", "trend", "terms"),
        terms = NULL, se.fit = TRUE, signif = 0.95, locations,
        variogram.model = NULL, param = NULL, aniso = NULL, variogram.object = NULL,
        control = control.predict.georob(), verbose = 0, ...)

control.predict.georob(full.covmat = FALSE, extended.output = FALSE,
                       mmax = 10000, ncores = pcmp[["max.ncores"]], pwidth = NULL, pheight = NULL,
                       napp = 1, pcmp = control.pcmp())
```

## Arguments

object	an object of class "georob" (mandatory argument), see <a href="#">georobObject</a> .
newdata	an optional data frame, <a href="#">SpatialPointsDataFrame</a> , <a href="#">SpatialPixelsDataFrame</a> , <a href="#">SpatialGridDataFrame</a> , <a href="#">SpatialPolygonsDataFrame</a> or an (optional) object of class <a href="#">SpatialPoints</a> , <a href="#">SpatialPixels</a> or <a href="#">SpatialGrid</a> , in which to look for variables with which to compute fitted values or Kriging predictions, see <i>Details</i> . If newdata is a <a href="#">SpatialPolygonsDataFrame</a> then block Kriging predictions are computed, otherwise point Kriging predictions.
type	a character keyword defining what target quantity should be predicted (computed). Possible values are <ul style="list-style-type: none"> <li>"signal": the "signal" <math>Z(\mathbf{s}) = \mathbf{x}(\mathbf{s})^T \boldsymbol{\beta} + B(\mathbf{s})</math> of the process (default),</li> <li>"response": the observations <math>Y(\mathbf{s}) = Z(\mathbf{s}) + \varepsilon(\mathbf{s})</math>,</li> <li>"trend": the external drift <math>\mathbf{x}(\mathbf{s})^T \boldsymbol{\beta}</math>,</li> <li>"terms": the model terms.</li> </ul>
terms	If type = "terms", which terms (default is all terms).
se.fit	a logical scalar, only used if type is equal to "terms", see <a href="#">predict.lm</a> .
signif	a positive numeric scalar equal to the tolerance or confidence level for computing respective intervals. If NULL no intervals are computed.
locations	an optional one-sided formula specifying what variables of newdata are the coordinates of the prediction points (default: <code>object[["locations.objects"]][["locations"]]</code> ).

variogram.model	an optional character keyword defining the variogram model to be used for Kriging, see <a href="#">georob</a> and <i>Details</i> .
param	an optional named numeric vector with values of the variogram parameters used for Kriging, see <a href="#">georob</a> and <i>Details</i> .
aniso	an optional named numeric vector with values of anisotropy parameters of a variogram used for Kriging, see <a href="#">georob</a> and <i>Details</i> .
variogram.object	an optional list that defines a possibly nested variogram model used for Kriging, see <a href="#">georob</a> and <i>Details</i> .
control	a list with the components <code>full.covmat</code> , <code>extended.output</code> , <code>mmax</code> , <code>ncores</code> , <code>pwidth</code> , <code>pheight</code> , <code>napp</code> and <code>pcmp</code> or a function such as <code>control.predict.georob</code> that generates such a list.
full.covmat	a logical scalar controlling whether the full covariance matrix of the prediction errors is returned (TRUE) or only the vector with its diagonal elements (FALSE, default), see <i>Value</i> for an explanation of the effect of <code>full.covmat</code> .
extended.output	a logical scalar controlling whether the covariance matrices of the Kriging predictions and of the data should be computed, see <i>Details</i> (default FALSE).
mmax	a positive integer equal to the maximum number (default 10000) of prediction items, computed in a sub-task in parallelized computations, see <i>Details</i> .
ncores	a positive integer controlling how many cores are used for parallelized computations, see <i>Details</i> .
pwidth, pheight, napp	numeric scalars, used to tune numeric integration of semi-variances for block Kriging, see <a href="#">preCKrige</a> .
pcmp	a list of arguments passed to <a href="#">pmm</a> and other functions that carry out parallelized computations or a function such as <code>control.pcmp</code> that generates such a list (see <code>control.pcmp</code> for allowed arguments).
verbose	a positive integer controlling logging of diagnostic messages to the console. <code>verbose = 0</code> (default) largely suppresses such messages.
...	arguments passed to <code>control.predict.georob</code> .

## Details

If `newdata` is an object of class `SpatialPoints`, `SpatialPixels` or `SpatialGrid` then the drift model may only use the coordinates as covariates (universal Kriging). Furthermore the names used for the coordinates in `newdata` must be the same as in `data` when creating object (argument `locations` of `predict.georob` should not be used). Note that the result returned by `predict.georob` is then an object of class `SpatialPointsDataFrame`, `SpatialPixelsDataFrame` or `SpatialGridDataFrame`.

The `predict` method for class `georob` uses the packages **parallel** and **snowfall** for parallelized computation of Kriging predictions. If there are  $m$  items to predict, the task is split into  $\text{ceiling}(m/mmax)$  sub-tasks that are then distributed to `ncores` CPUs. Evidently, `ncores = 1` suppresses parallel execution. By default, the function uses all available CPUs as returned by [detectCores](#).

Note that if `full.covmat` is TRUE `mmax` must exceed  $m$  (and parallel execution is not possible).

The argument `extended.output = TRUE` is used to compute all quantities required for (approximately) unbiased back-transformation of Kriging predictions of log-transformed data to the original scale of the measurements by [lgnpp](#). In more detail, the following items are computed:

- `trend`: the fitted values,  $\mathbf{x}(\mathbf{s})^T \hat{\boldsymbol{\beta}}$ ,
- `var.pred`: the variances of the Kriging predictions,  $\text{Var}_{\hat{\theta}}[\hat{Y}(\mathbf{s})]$  or  $\text{Var}_{\hat{\theta}}[\hat{Z}(\mathbf{s})]$ ,
- `cov.pred.target`: the covariances between the predictions and the prediction targets,  $\text{Cov}_{\hat{\theta}}[\hat{Y}(\mathbf{s}), Y(\mathbf{s})]$  or  $\text{Cov}_{\hat{\theta}}[\hat{Z}(\mathbf{s}), Z(\mathbf{s})]$ ,
- `var.target`: the variances of the prediction targets  $\text{Var}_{\hat{\theta}}[Y(\mathbf{s})]$  or  $\text{Var}_{\hat{\theta}}[Z(\mathbf{s})]$ .

Note that the component `var.pred` is also present if `type` is equal to "trend", irrespective of the choice for `extended.output`. This component contains then the variances of the fitted values.

## Value

The method `predict.georob` returns, depending on its arguments, the following objects:

If `type` is equal to "terms" then a vector, a matrix, or a list with prediction results along with bounds and standard errors, see [predict.lm](#). Otherwise, the structure and contents of the output generated by `predict.georob` are determined by the class of `newdata` and the logical flags `full.covmat` and `extended.output`:

If `full.covmat` is FALSE then the result is an object of a "similar" class as `newdata` (data frame, [SpatialPointsDataFrame](#), [SpatialPixelsDataFrame](#), [SpatialGridDataFrame](#), [SpatialPolygonsDataFrame](#)).

The data frame or the data slot of the `Spatial...DataFrame` objects have the following components:

- the coordinates of the prediction points (only present if `newdata` is a data frame).
- `pred`: the Kriging predictions (or fitted values).
- `se`: the root mean squared prediction errors (Kriging standard errors).
- `lower`, `upper`: the limits of tolerance/confidence intervals,
- `trend`, `var.pred`, `cov.pred.target`, `var.target`: only present if `extended.output` is TRUE, see *Details*.

If `full.covmat` is TRUE then `predict.georob` returns a list with the following components:

- `pred`: a data frame or a `Spatial...DataFrame` object as described above for `full.covmat = FALSE`.
- `mse.pred`: the full covariance matrix of the prediction errors,  $Y(\mathbf{s}) - \hat{Y}(\mathbf{s})$  or  $Z(\mathbf{s}) - \hat{Z}(\mathbf{s})$  see *Details*.
- `var.pred`: the full covariance matrix of the Kriging predictions, see *Details*.
- `cov.pred.target`: the full covariance matrix of the predictions and the prediction targets, see *Details*.
- `var.target`: the full covariance matrix of the prediction targets, see *Details*.

The function `control.predict.georob` returns a list with control parameters to steer `predict.georob`, see arguments of the function above for its components.

**Author(s)**

Andreas Papritz <papritz@retired.ethz.ch>.

**References**

Nussbaum, M., Papritz, A., Baltensweiler, A. and Walthert, L. (2014) Estimating soil organic carbon stocks of Swiss forest soils by robust external-drift kriging. *Geoscientific Model Development*, **7**, 1197–1210. doi:10.5194/gmd711972014.

Künsch, H. R., Papritz, A., Schwierz, C. and Stahel, W. A. (2011) Robust estimation of the external drift and the variogram of spatial data. Proceedings of the ISI 58th World Statistics Congress of the International Statistical Institute. doi:10.3929/ethza009900710

**See Also**

[georobPackage](#) for a description of the model and a brief summary of the algorithms;  
[georob](#) for (robust) fitting of spatial linear models;  
[georobObject](#) for a description of the class georob;  
[profilelogLik](#) for computing profiles of Gaussian likelihoods;  
[plot.georob](#) for display of RE(ML) variogram estimates;  
[control.georob](#) for controlling the behaviour of georob;  
[georobModelBuilding](#) for stepwise building models of class georob;  
[cv.georob](#) for assessing the goodness of a fit by georob;  
[georobMethods](#) for further methods for the class georob;  
[lgnpp](#) for unbiased back-transformation of Kriging prediction of log-transformed data;  
[georobSimulation](#) for simulating realizations of a Gaussian process from model fitted by georob;  
 and finally  
[sample.variogram](#) and [fit.variogram.model](#) for robust estimation and modelling of sample variograms.

**Examples**

```
data(meuse)

data(meuse.grid)
coordinates(meuse.grid) <- ~x+y
meuse.grid.pixdf <- meuse.grid
gridded(meuse.grid.pixdf) <- TRUE

data(meuse.blocks, package = "constrainedKriging")

r.logzn.rob <- georob(log(zinc) ~ sqrt(dist), data = meuse, locations = ~ x + y,
  variogram.model = "RMexp", param = c(variance = 0.15, nugget = 0.05, scale = 200),
  tuning.psi = 1., control = control.georob(cov.bhat = TRUE, full.cov.bhat = TRUE))

## point predictions of log(Zn)
r.pred.points.1 <- predict(r.logzn.rob, newdata = meuse.grid.pixdf,
```



```

    control = control.predict.georob(extended.output = TRUE))
str(r.pred.points.1, max = 3)

## back-transformation of point predictions
r.backtf.pred.points <- lgnpp(r.pred.points.1)
str(r.backtf.pred.points, max = 3)

spplot(r.backtf.pred.points, zcol = "lgn.pred", main = "Zn content")

## predicting mean Zn content for whole area
if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s
  ## recompute point predictions with argument full.covmat = TRUE
  r.pred.points.2 <- predict(r.logzn.rob, newdata = meuse.grid.pixdf,
    control = control.predict.georob(extended.output = TRUE, full.covmat = TRUE))
  str(r.pred.points.2, max = 3)
  r.block <- lgnpp(r.pred.points.2, is.block = TRUE, all.pred = r.backtf.pred.points@data)
  r.block
}

## block predictions of log(Zn)
if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s
  r.pred.block <- predict(r.logzn.rob, newdata = meuse.blocks,
    control = control.predict.georob(extended.output = TRUE,
      pwidth = 75, pheight = 75, mmax = 50))
  r.backtf.pred.block <- lgnpp(r.pred.block, newdata = meuse.grid)

  spplot(r.backtf.pred.block, zcol = "lgn.pred", main = "block means Zn content")
}

```

---

profilelogLik

*Profile Likelihood*


---

### Description

The function `profilelogLik` computes for an array of fixed variogram parameters the profile log-likelihood by maximizing the (restricted) log-likelihood with respect to the remaining variogram parameters, the fixed and random effects.

### Usage

```

profilelogLik(object, values, use.fitted = TRUE, verbose = 0,
  ncores = min(parallel::detectCores(), NROW(values)))

```

### Arguments

`object` an object of class "georob" (mandatory argument), see [georobObject](#).

values	a <code>data.frame</code> or a matrix with the values of the variogram and anisotropy parameters that should be kept fixed (mandatory argument, see <a href="#">georob</a> and <a href="#">georobPackage</a> for information about the parametrization of variogram models). The names of the columns of values must match the names of variogram and anisotropy parameters.
use.fitted	a logical scalar controlling whether the fitted variogram parameters of object should be used as initial values (default TRUE) when maximizing the profile log-likelihood or the initial values used to generate object.
verbose	a positive integer controlling logging of diagnostic messages to the console during model fitting, see <a href="#">georob</a> .
ncores	a positive integer controlling how many cores are used for parallelized computations, see <i>Details</i> .

### Details

For robust REML fits `profilelogLik` returns (possibly with a warning) the log-likelihood of the Gaussian (RE)ML fit of the equivalent Gaussian spatial linear model with heteroscedastic nugget.

**Note** that *the data frame passed as data argument to georob must exist in the user workspace when calling profilelogLik*.

`profilelogLik` uses the packages **parallel** and **snowfall** for parallelized computation of the profile likelihood. By default, the function uses `NROW(values)` CPUs but not more than are physically available (as returned by [detectCores](#)).

`profilelogLik` uses the function [update](#) to re-estimated the model with partly fixed variogram parameters. Therefore, any argument accepted by [georob](#) except `data` can be changed when re-fitting the model. Some of them (e.g. `verbose`) are explicit arguments of `profilelogLik`, but also the remaining ones can be passed by `...` to the function.

### Value

A `data.frame` with the columns of values, a column `logLik` (contains the maximized [restricted] log-likelihood), columns with the estimated variogram and fixed effect parameters, columns with the gradient of the (restricted) log-likelihood (or the roots of the estimating equations) and a column `converged`, indicating whether convergence has occurred when fitting the respective model.

### Author(s)

Andreas Papritz <[papritz@retired.ethz.ch](mailto:papritz@retired.ethz.ch)>.

### See Also

[georobPackage](#) for a description of the model and a brief summary of the algorithms;

[georob](#) for (robust) fitting of spatial linear models;

[georobObject](#) for a description of the class `georob`;

[plot.georob](#) for display of RE(ML) variogram estimates;

[control.georob](#) for controlling the behaviour of `georob`;

[georobModelBuilding](#) for stepwise building models of class `georob`;

[cv.georob](#) for assessing the goodness of a fit by georob;  
[georobMethods](#) for further methods for the class georob;  
[predict.georob](#) for computing robust Kriging predictions;  
[lgnpp](#) for unbiased back-transformation of Kriging prediction of log-transformed data;  
[georobSimulation](#) for simulating realizations of a Gaussian process from model fitted by georob;  
 and finally  
[sample.variogram](#) and [fit.variogram.model](#) for robust estimation and modelling of sample variograms.

## Examples

```

## define number of cores for parallel computations
if(interactive()) ncpu <- 2L else ncpu <- 1L

data(meuse)

r.logzn.ml <- georob(log(zinc)~sqrt(dist), data=meuse, locations=~x+y,
  variogram.model="RMexp", param=c(variance=0.15, nugget=0.05, scale=200),
  tuning.psi=1000, control=control.georob(ml.method="ML"))

if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s
  r.prflik <- profilelogLik(r.logzn.ml, values=expand.grid(scale=seq(75, 600, by=25)),
    ncores = ncpu)

  plot(loglik~scale, r.prflik, type="l")
  abline(v=r.logzn.ml$variogram.object[[1]]$param["scale"], lty="dotted")
  abline(h=r.logzn.ml$loglik-0.5*qchisq(0.95, 1), lty="dotted")
}

```

---

 reexported-fun

*Re-Exported Functions from R package imports*


---

## Description

The imported functions [K](#), [lmrob.control](#), and [waldtest](#) are re-exported for ease of use without attaching the respective packages.

## Usage

```
K(dist, model)
```

```

lmrob.control(setting, seed = NULL, nResample = 500, tuning.chi = NULL,
  bb = 0.5, tuning.psi = NULL, max.it = 50, groups = 5, n.group = 400,
  k.fast.s = 1, best.r.s = 2, k.max = 200, maxit.scale = 200, k.m_s = 20,
  refine.tol = 1e-7, rel.tol = 1e-7, scale.tol = 1e-10, solve.tol = 1e-7,
  zero.tol = 1e-10, trace.lev = 0, mts = 1000,

```

```

subsampling = c("nonsingular", "simple"), compute.rd = FALSE,
method = "MM", psi = "bisquare", numpoints = 10, cov = NULL,
split.type = c("f", "fi", "fii"), fast.s.large.n = 2000,
# only for outlierStats() :
eps.outlier = function(nobs) 0.1 / nobs,
eps.x = function(maxx) .Machine$double.eps^(.75)*maxx,
compute.outlier.stats = method, warn.limit.reject = 0.5,
warn.limit.meanrw = 0.5, ...)

```

## Arguments

<code>dist</code>	a numeric vector with distances.
<code>model</code>	an object of class “covmodel” that defines an isotropic covariance model, see <a href="#">covmodel</a> .
<code>setting</code>	a string specifying alternative default values, see <a href="#">lmrob.control</a> .
<code>seed</code>	NULL or an integer vector compatible with <a href="#">.Random.seed</a> , see <a href="#">lmrob.control</a> .
<code>nResample</code>	number of re-sampling candidates to be used to find the initial S-estimator, see <a href="#">lmrob.control</a> .
<code>tuning.chi</code>	tuning constant vector for the S-estimator, see <a href="#">lmrob.control</a> .
<code>bb</code>	expected value under the normal model of the “chi”, see <a href="#">lmrob.control</a>
<code>tuning.psi</code>	tuning constant vector for the redescending M-estimator, see <a href="#">lmrob.control</a> .
<code>max.it</code>	integer specifying the maximum number of IRWLS iterations, see <a href="#">lmrob.control</a> .
<code>groups</code>	(for the fast-S algorithm): Number of random subsets to use when the data set is large, see <a href="#">lmrob.control</a> .
<code>n.group</code>	(for the fast-S algorithm): Size of each of the groups above, see <a href="#">lmrob.control</a> .
<code>k.fast.s</code>	(for the fast-S algorithm): Number of local improvement steps (“I-steps”) for each re-sampling candidate, see <a href="#">lmrob.control</a> .
<code>best.r.s</code>	(for the fast-S algorithm): Number of of best candidates to be iterated further, see <a href="#">lmrob.control</a> .
<code>k.max</code>	(for the fast-S algorithm): maximal number of refinement steps for the “fully” iterated best candidates, see <a href="#">lmrob.control</a> .
<code>maxit.scale</code>	integer specifying the maximum number of C level <code>find_scale()</code> iterations (in fast-S and M-S algorithms), see <a href="#">lmrob.control</a> .
<code>k.m_s</code>	(for the M-S algorithm): specifies after how many unsuccessful refinement steps the algorithm stops, see <a href="#">lmrob.control</a> .
<code>refine.tol</code>	(for the fast-S algorithm): relative convergence tolerance for the fully iterated best candidates, see <a href="#">lmrob.control</a> .
<code>rel.tol</code>	(for the RWLS iterations of the MM algorithm): relative convergence tolerance for the parameter vector, see <a href="#">lmrob.control</a> .
<code>scale.tol</code>	(for the scale estimation iterations of the S algorithm): relative convergence tolerance for the scale $\sigma(\cdot)$ , see <a href="#">lmrob.control</a> , see <a href="#">lmrob.control</a> .
<code>solve.tol</code>	(for the S algorithm): relative tolerance for inversion see <a href="#">lmrob.control</a> .

<code>zero.tol</code>	for checking 0-residuals in the S algorithm, non-negative number, see <a href="#">lmrob.control</a> .
<code>trace.lev</code>	integer indicating if the progress of the MM-algorithm and the fast-S algorithms should be traced, see <a href="#">lmrob.control</a> .
<code>mts</code>	maximum number of samples to try in subsampling algorithm, see <a href="#">lmrob.control</a> .
<code>subsampling</code>	type of subsampling to be used, see <a href="#">lmrob.control</a> .
<code>compute.rd</code>	a logical scalar indicating if robust distances (based on the MCD robust covariance estimator) are to be computed for the robust diagnostic plots, see <a href="#">lmrob.control</a> .
<code>method</code>	string specifying the estimator-chain, see <a href="#">lmrob.control</a> .
<code>psi</code>	string specifying the type $\psi$ -function used., see <a href="#">lmrob.control</a> .
<code>numpoints</code>	number of points used in Gauss quadrature, see <a href="#">lmrob.control</a>
<code>cov</code>	function or string with function name to be used to calculate covariance matrix estimate, see <a href="#">lmrob.control</a> .
<code>split.type</code>	determines how categorical and continuous variables are split, see <a href="#">lmrob.control</a> .
<code>fast.s.large.n</code>	minimum number of observations required to switch from ordinary “fast S” algorithm to an efficient “large n” strategy, see <a href="#">lmrob.control</a>
<code>eps.outlier</code>	limit on the robustness weight below which an observation is considered to be an outlier, see <a href="#">lmrob.control</a> .
<code>eps.x</code>	limit on the absolute value of the elements of the design matrix below which an element is considered zero, see <a href="#">lmrob.control</a> .
<code>compute.outlier.stats</code>	vector of character strings, each valid to be used as method argument, see <a href="#">lmrob.control</a>
<code>warn.limit.reject</code>	see <a href="#">lmrob.control</a> .
<code>warn.limit.meanrw</code>	limit of the mean robustness per factor level below which ( $\leq$ ) a warning is produced. Set to NULL to disable warning.
<code>...</code>	some methods for the generic function <a href="#">waldtest</a> require additional arguments, see respective help pages.

## Details

The function [K](#) is required for computing block Kriging predictions by the function [f.point.block.cov](#) of the package **constrainedKriging**.

Furthermore, the function [lmrob.control](#) allows to pass tuning parameters to the function [lmrob](#) of the package **robustbase**, which is used for computing robust initial values of the regression coefficients.

## Value

See help pages of [K](#) and [lmrob.control](#) for the output generated by these functions.

**Description**

The function `sample.variogram` computes the sample (empirical) variogram of a spatial variable by the method-of-moment and three robust estimators. Both omnidirectional and direction-dependent variograms can be computed, the latter for observation locations in a three-dimensional domain. There are summary and plot methods for summarizing and displaying sample variograms.

**Usage**

```
sample.variogram(object, ...)

## Default S3 method:
sample.variogram(object, locations, lag.dist.def,
  xy.angle.def = c(0, 180), xz.angle.def = c(0, 180), max.lag = Inf,
  estimator = c("qn", "mad", "matheron", "ch"), mean.angle = TRUE, ...)

## S3 method for class 'formula'
sample.variogram(object, data, subset, na.action,
  locations, lag.dist.def, xy.angle.def = c(0, 180),
  xz.angle.def = c(0, 180), max.lag = Inf,
  estimator = c("qn", "mad", "matheron", "ch"), mean.angle = TRUE, ...)

## S3 method for class 'georob'
sample.variogram(object, lag.dist.def,
  xy.angle.def = c(0, 180), xz.angle.def = c(0, 180), max.lag = Inf,
  estimator = c("qn", "mad", "matheron", "ch"), mean.angle = TRUE, ...)

## S3 method for class 'sample.variogram'
summary(object, ...)

## S3 method for class 'sample.variogram'
plot(x, type = "p", add = FALSE,
  xlim = c(0, max(x[["lag.dist"]])),
  ylim = c(0, 1.1 * max(x[["gamma"]])), col, pch, lty, cex = 0.8,
  xlab = "lag distance", ylab = "semivariance",
  annotate.npairs = FALSE, npairs.pos = 3, npairs.cex = 0.7,
  legend = nlevels(x[["xy.angle"]]) > 1 || nlevels(x[["xz.angle"]]) > 1,
  legend.pos = "topleft", ...)
```

**Arguments**

`object` a numeric vector with the values of the response for which the sample variogram should be computed (`sample.variogram.default`), a formula, specifying in its left part the response variable (right part of formula is ignored,

	sample.variogram.formula), an object of class <code>georob</code> ( <code>sample.variogram.georob</code> ) or an object of class <code>sample.variogram.summary.sample.variogram</code> ).
locations	a numeric matrix with the coordinates of the locations where the response was observed ( <code>sample.variogram.default</code> ) or a one-sided formula specifying the coordinates ( <code>sample.variogram.formula</code> ). The matrix may have an arbitrary number of columns for an omnidirectional variogram, but at most 3 columns if a directional variogram is computed.
data	an optional data frame, list or environment (or another object coercible by <code>as.data.frame</code> to a data frame) containing the response variable and the coordinates where the data was recorded. If not found in <code>data</code> , the variables are taken from <code>environment(formula)</code> , typically the environment from which <code>sample.variogram</code> is called.
subset	an optional vector specifying a subset of observations to be used for estimating the variogram.
na.action	a function which indicates what should happen when the data contain NAs. The default is set by the <code>na.action</code> argument of <code>options</code> , and is <code>na.fail</code> if that is unset. The “factory-fresh” default is <code>na.omit</code> . Another possible value is <code>NULL</code> , no action. Value <code>na.exclude</code> can be useful.
lag.dist.def	a numeric scalar defining a constant bin width for grouping the lag distances or a numeric vector with the bounds of a set of contiguous bins (upper bounds of bins except for the first element of <code>lag.dist.def</code> which is the lower bound of the first bin). This argument is mandatory.
xy.angle.def	an numeric vector defining angular classes in the horizontal plane for computing directional variograms. <code>xy.angle.def</code> must contain an ascending sequence of azimuth angles in degrees from north (positive clockwise to south), see <i>Details</i> . Omnidirectional variograms are computed with the default <code>c(0, 180)</code> .
xz.angle.def	an numeric vector defining angular classes in the <i>x-z</i> -plane for computing directional variograms. <code>xz.angle.def</code> must contain an ascending sequence of angles in degrees from zenith (positive clockwise to nadir), see <i>Details</i> . Omnidirectional variograms are computed with the default <code>c(0, 180)</code> .
max.lag	a positive numeric defining the largest lag distance for which semi variances should be computed (default no restriction).
estimator	a character keyword defining the estimator for computing the sample variogram. Possible values are: <ul style="list-style-type: none"> <li>• “qn”: Genton’s robust <math>Q_n</math>-estimator (default, <i>Genton, 1998</i>),</li> <li>• “mad”: Dowd’s robust MAD-estimator (<i>Dowd, 1984</i>),</li> <li>• “matheron”: non-robust method-of-moments estimator,</li> <li>• “ch”: robust Cressie-Hawkins estimator (<i>Cressie and Hawkins, 1980</i>).</li> </ul>
mean.angle	a logical scalar controlling whether the mean lag vector (per combination of lag distance and angular class) is computed from the mean angles of all the lag vectors falling into a given class ( <code>TRUE</code> , default) or from the mid-angles of the respective angular classes ( <code>FALSE</code> ).
x	an object of class <code>sample.variogram</code> .

type, xlim, ylim, xlab, ylab	see respective arguments of <code>plot.default</code> .
add	a logical scalar controlling whether a new plot should be generated (FALSE, default) or whether the information should be added to the current plot (TRUE).
col	a vector with the colours of plotting symbols for distinguishing semi variances for angular classes in the $x$ - $y$ -plane.
pch	a vector with the types of plotting symbols for distinguishing semi variances for angular classes in the $x$ - $z$ -plane.
lty	the line type.
cex	a numeric with the character expansion factor for plotting symbols.
annotate.npairs	a logical scalar controlling whether the plotting symbols should be annotated by the number of data pairs per lag class.
npairs.pos	an integer defining the position where text annotation about number of pairs should be plotted, see <code>text</code> .
npairs.cex	a numeric defining the character expansion for text annotation about number of pairs.
legend	a logical scalar controlling whether a <code>legend</code> should be plotted.
legend.pos	a character keyword defining where to place the legend, see <code>legend</code> for possible values.
...	additional arguments passed to <code>plot.formula</code> .

## Details

The angular classes in the  $x$ - $y$ - and  $x$ - $z$ -plane are defined by vectors of ascending angles on the half circle. The  $i$ th angular class is defined by the vector elements, say  $l$  and  $u$ , with indices  $i$  and  $i + 1$ . A lag vector belongs to the  $i$ th angular class if its azimuth (or angle from zenith), say  $\varphi$ , satisfies  $l < \varphi \leq u$ . If the first and the last element of `xy.angle.def` or `xz.angle.def` are equal to  $0$  and  $180$  degrees, respectively, then the first and the last angular class are “joined”, i.e., if there are  $K$  angles, there will be only  $K - 2$  angular classes and the first class is defined by the interval ( `xy.angle.def[K-1]-180`, `xy.angle.def[2]` ] and the last class by ( `xy.angle.def[K-2]`, `xy.angle.def[K-1]`].

## Value

All methods of the generic function `sample.variogram` return an object of class `sample.variogram`, which is a data frame with the following components:

<code>lag.dist</code>	the mean lag distance of the lag class,
<code>xy.angle</code>	the angular class in the $x$ - $y$ -plane,
<code>xz.angle</code>	the angular class in the $x$ - $z$ -plane,
<code>gamma</code>	the estimated semi-variance of the lag class,
<code>npairs</code>	the number of data pairs in the lag class,
<code>lag.x</code>	the $x$ -component of the mean lag vector of the lag class,
<code>lag.y</code>	the $y$ -component of the mean lag vector of the lag class,
<code>lag.z</code>	the $z$ -component of the mean lag vector of the lag class.



The method `summary.sample.variogram` returns an object of class `summary.sample.variogram` which is list with the components `log.dist`, `npairs`, `xy.angle` and `xz.angle`, see description for object of class `sample.variogram` above. There is a `print` method for objects of class `summary.sample.variogram` which invisibly returns the object unchanged.

The method `plot.sample.variogram` is called for its side effects and invisibly returns the object `sample.variogram` unchanged.

### Author(s)

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### References

Cressie, N. and Hawkins, D. M. (1980) Robust Estimation of the Variogram: I. *Mathematical Geology*, **12**, 115–125, doi:10.1007/BF01035243.

Dowd, P. A. (1984) The variogram and Kriging: Robust and resistant estimators. In *Geostatistics for Natural Resources Characterization*, Verly, G., David, M., Journel, A. and Marechal, A. (Eds.) Dordrecht: D. Reidel Publishing Company, Part I, 1, 91–106, doi:10.1007/9789400936997.

Genton, M. (1998) Highly Robust Variogram Estimation. *Mathematical Geology*, **30**, 213–220, doi:10.1023/A:1021728614555.

### See Also

[georobPackage](#) for a description of the model and a brief summary of the algorithms;  
[georob](#) for (robust) fitting of spatial linear models;  
[georobObject](#) for a description of the class `georob`;  
[profilelogLik](#) for computing profiles of Gaussian likelihoods;  
[plot.georob](#) for display of RE(ML) variogram estimates;  
[control.georob](#) for controlling the behaviour of `georob`;  
[georobModelBuilding](#) for stepwise building models of class `georob`;  
[cv.georob](#) for assessing the goodness of a fit by `georob`;  
[georobMethods](#) for further methods for the class `georob`;  
[predict.georob](#) for computing robust Kriging predictions;  
[lgnpp](#) for unbiased back-transformation of Kriging prediction of log-transformed data;  
[georobSimulation](#) for simulating realizations of a Gaussian process from model fitted by `georob`.

### Examples

```
data(wolfcamp)

## omnidirectional sample variogram
r.sv.iso <- sample.variogram(pressure~1, data = wolfcamp,
  locations = ~x + y, lag.dist.def = seq(0, 200, by = 15))
```

```

plot(r.sv.iso, type = "l")

## direction-dependent sample variogram
r.sv.aniso <- sample.variogram(pressure~1, data = wolfcamp,
  locations = ~x + y, lag.dist.def = seq(0, 200, by = 15),
  xy.angle.def = c(0., 22.5, 67.5, 112.5, 157.5, 180.))
plot(r.sv.aniso, type = "l", add = TRUE, col = 2:5)

```

---

validate.predictions *Summary Statistics of (Cross-)Validation Prediction Errors*

---

## Description

Functions to compute and plot summary statistics of prediction errors to (cross-)validate fitted spatial linear models by the criteria proposed by *Gneiting et al. (2007)* for assessing probabilistic forecasts.

## Usage

```

validate.predictions(data, pred, se.pred,
  statistic = c("crps", "pit", "mc", "bs", "st"), ncutoff = NULL)

## S3 method for class 'cv.georob'
plot(x,
  type = c("sc", "lgn.sc", "ta", "qq", "hist.pit", "ecdf.pit", "mc", "bs"),
  smooth = TRUE, span = 2/3, ncutoff = NULL, add = FALSE,
  col, pch, lty, main, xlab, ylab, ...)

## S3 method for class 'cv.georob'
print(x, digits = max(3, getOption("digits") - 3), ...)

## S3 method for class 'cv.georob'
summary(object, se = FALSE, ...)

```

## Arguments

data	a numeric vector with observations about a response (mandatory argument).
pred	a numeric vector with predictions for the response (mandatory argument).
se.pred	a numeric vector with prediction standard errors (mandatory argument).
statistic	a character keyword defining what statistic of the prediction errors should be computed. Possible values are (see <i>Details</i> ): <ul style="list-style-type: none"> <li>• "crps": continuous ranked probability score (default),</li> <li>• "pit": probability integral transform,</li> <li>• "mc": average predictive distribution (marginal calibration),</li> <li>• "bs": Brier score,</li> </ul>

	<ul style="list-style-type: none"> <li>• "st": mean and dispersion statistics of (standardized) prediction errors.</li> </ul>
ncutoff	a positive integer ( $N$ ) giving the number of quantiles, for which CDFs are evaluated (type = "mc"), or the number of thresholds for which the Brier score is computed (type = "bs"), see <i>Details</i> (default: $\min(500, \text{length}(\text{data}))$ ).
x, object	objects of class <code>cv.georob</code> .
digits	a positive integer indicating the number of decimal digits to print.
type	a character keyword defining what type of plot is created by the <code>plot.cv.georob</code> . Possible values are: <ul style="list-style-type: none"> <li>• "sc": a scatter-plot of the (possibly log-transformed) response vs. the respective predictions (default).</li> <li>• "lgn.sc": a scatter-plot of the untransformed response against back-transformed predictions of the log-transformed response.</li> <li>• "ta": Tukey-Anscombe plot (plot of standardized prediction errors vs. predictions).</li> <li>• "qq": normal QQ plot of standardized prediction errors.</li> <li>• "hist.pit": histogram of probability integral transform, see <i>Details</i>.</li> <li>• "ecdf.pit": empirical CDF of probability integral transform, see <i>Details</i>.</li> <li>• "mc": a marginal calibration plot, see <i>Details</i>,</li> <li>• "bs": a plot of Brier score vs. threshold, see <i>Details</i>.</li> </ul>
smooth	a logical scalar controlling whether scatter plots of data vs. predictions should be smoothed by <a href="#">loess.smooth</a> .
span	a numeric with the smoothness parameter for loess (see <a href="#">loess.smooth</a> ).
add	a logical scalar controlling whether the current high-level plot is added to an existing graphics without cleaning the frame before (default: FALSE).
main, xlab, ylab	title and axes labels of plot.
col, pch, lty	color, symbol and line type.
se	a logical scalar controlling if the standard errors of the averaged continuous ranked probability score and of the mean and dispersion statistics of the prediction errors (see <i>Details</i> ) are computed from the respective values of the $K$ cross-validation subsets (default: FALSE).
...	additional arguments passed to the methods.

## Details

`validate.predictions` computes the items required to evaluate (and plot) the diagnostic criteria proposed by *Gneiting et al. (2007)* for assessing the *calibration* and the *sharpness* of probabilistic predictions of (cross-)validation data. To this aim, `validate.predictions` uses the assumption that the prediction errors  $Y(s) - \hat{Y}(s)$  follow normal distributions with zero mean and standard deviations equal to the Kriging standard errors. This assumption is an approximation if the errors  $\varepsilon$  come from a long-tailed distribution. Furthermore, for the time being, the Kriging variance of the response  $Y$  is approximated by adding the estimated nugget  $\hat{\tau}^2$  to the Kriging variance of the signal  $Z$ . This approximation likely underestimates the mean squared prediction error of the response if the errors come from a long-tailed distribution. Hence, for robust Kriging, the standard errors of the (cross-)validation errors are likely too small.

Notwithstanding these difficulties and imperfections, `validate.predictions` computes

- the *probability integral transform* (PIT),

$$\text{PIT}_i = F_i(y_i),$$

where  $F_i(y_i)$  denotes the (plug-in) predictive CDF evaluated at  $y_i$ , the value of the  $i$ th (cross-)validation datum,

- the *average predictive CDF* (plug-in)

$$\bar{F}_n(y) = 1/n \sum_{i=1}^n F_i(y),$$

where  $n$  is the number of (cross-)validation observations and the  $F_i$  are evaluated at  $N$  quantiles equal to the set of distinct  $y_i$  (or a subset of size  $N$  of them),

- the *Brier Score* (plug-in)

$$\text{BS}(y) = 1/n \sum_{i=1}^n (F_i(y) - I(y_i \leq y))^2,$$

where  $I(x)$  is the indicator function for the event  $x$ , and the Brier score is again evaluated at the unique values of the (cross-)validation observations (or a subset of size  $N$  of them),

- the *averaged continuous ranked probability score*, CRPS, a strictly proper scoring criterion to rank predictions, which is related to the Brier score by

$$\text{CRPS} = \int_{-\infty}^{\infty} \text{BS}(y) dy.$$

Gneiting et al. (2007) proposed the following plots to validate probabilistic predictions:

- A histogram (or a plot of the empirical CDF) of the PIT values. For ideal predictions, with observed coverages of prediction intervals matching nominal coverages, the PIT values have a uniform distribution.
- Plots of  $\bar{F}_n(y)$  and of the empirical CDF of the data, say  $\hat{G}_n(y)$ , and of their difference,  $\bar{F}_n(y) - \hat{G}_n(y)$  vs  $y$ . The forecasts are said to be *marginally calibrated* if  $\bar{F}_n(y)$  and  $\hat{G}_n(y)$  match.
- A plot of  $\text{BS}(y)$  vs.  $y$ . Probabilistic predictions are said to be *sharp* if the area under this curve, which equals CRPS, is minimized.

The `plot` method for class `cv.georob` allows to create these plots, along with scatter-plots of observations and predictions, Tukey-Anscombe and normal QQ plots of the standardized prediction errors.

`summary.cv.georob` computes the mean and dispersion statistics of the (standardized) prediction errors (by a call to `validate.prediction` with argument `statistic = "st"`, see *Value*) and the averaged continuous ranked probability score (`crps`). If present in the `cv.georob` object, the error statistics are also computed for the errors of the unbiasedly back-transformed predictions of a log-transformed response. If `se` is TRUE then these statistics are evaluated separately for the  $K$  cross-validation subsets and the standard errors of the means of these statistics are returned as well.

The `print` method for class `cv.georob` returns the mean and dispersion statistics of the (standardized) prediction errors.

**Value**

Depending on the argument `statistic`, the function `validate.predictions` returns

- a numeric vector of PIT values if `statistic` is equal to "pit",
- a named numeric vector with summary statistics of the (standardized) prediction errors if `statistic` is equal to "st". The following statistics are computed:

me	mean prediction error
mede	median prediction error
rmse	root mean squared prediction error
made	median absolute prediction error
qne	Qn dispersion measure of prediction errors (see <a href="#">Qn</a> )
msse	mean squared standardized prediction error
medsse	median squared standardized prediction error

- a data frame if `statistic` is equal to "mc" or "bs" with the components (see *Details*):

z	the sorted unique (cross-)validation observations (or a subset of size <code>ncutoff</code> of them)
ghat	the empirical CDF of the (cross-)validation observations $\hat{G}_n(y)$
fbar	the average predictive distribution $\bar{F}_n(y)$
bs	the Brier score $BS(y)$

The method `print.cv.georob` invisibly returns the object unchanged.

The method `summary.cv.georob` returns an object of class `summary.cv.georob` which is a list with 3 components:

- `st` a numeric vector with summary statistics of the (standardized) prediction errors of the possibly log-transformed response, see output of function `validate.predictions` for argument `statistic = "st"` above.
- `crps` the value of the continuous ranked probability score.
- `st.lgn` a numeric vector with summary statistics of the (standardized) prediction errors of the back-transformed response if argument `lgn = TRUE` and `NULL` otherwise.

There is a `print` method for objects of class `summary.cv.georob` which invisibly returns the object unchanged.

The method `plot.georob` is called for its side effects and invisibly returns `NULL`.

**Author(s)**

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**References**

Gneiting, T., Balabdaoui, F. and Raftery, A. E. (2007) Probabilistic forecasts, calibration and sharpness. *Journal of the Royal Statistical Society Series B* **69**, 243–268, [doi:10.1111/j.14679868.2007.00587.x](https://doi.org/10.1111/j.14679868.2007.00587.x).

**See Also**

[georob](#) for (robust) fitting of spatial linear models;  
[cv.georob](#) for assessing the goodness of a fit by georob.

**Examples**

```
## define number of cores for parallel computations
if(interactive()) ncpu <- 10L else ncpu <- 1L

data(meuse)

r.logzn <- georob(log(zinc) ~ sqrt(dist), data = meuse, locations = ~ x + y,
  variogram.model = "RMexp",
  param = c(variance = 0.15, nugget = 0.05, scale = 200),
  tuning.psi = 1000)

if(interactive()){
  ## example is run only in interactive session because cpu times exceeds 5 s
  r.logzn.cv.1 <- cv(r.logzn, seed = 1, lgn = TRUE, ncores = 1, verbose = 1)

  r.logzn.cv.2 <- cv(r.logzn, formula = .~. + ffreq, seed = 1, lgn = TRUE,
    ncores = ncpu)

  summary(r.logzn.cv.1, se = TRUE)
  summary(r.logzn.cv.2, se = TRUE)

  op <- par(mfrow = c(2,2))
  plot(r.logzn.cv.1, type = "lgn.sc")
  plot(r.logzn.cv.2, type = "lgn.sc", add = TRUE, col = "red")
  abline(0, 1, lty= "dotted")
  plot(r.logzn.cv.1, type = "ta")
  plot(r.logzn.cv.2, type = "ta", add = TRUE, col = "red")
  abline(h=0, lty= "dotted")
  plot(r.logzn.cv.2, type = "mc", col = "red")
  plot(r.logzn.cv.1, type = "bs")
  plot(r.logzn.cv.2, type = "bs", add = TRUE, col = "red")
  legend("topright", lty = 1, col = c("black", "red"), bty = "n",
    legend = c("log(Zn) ~ sqrt(dist)", "log(Zn) ~ sqrt(dist) + ffreq"))
  par(op)
}
```

**Description**

Piezometric head measurements taken at the Wolfcamp Aquifer, Texas, USA. See *Cressie (1993, p. 212–214)* for description of the scientific problem and the data. Original data were converted to SI units: coordinates are given in kilometers and pressure heads in meters.

**Usage**

```
data(wolfcamp)
```

**Format**

A data frame with 85 observations on the following 3 variables:

x a numeric vector with the easting coordinate in kilometers.

y a numeric vector with the northing coordinate in kilometers.

pressure a numeric vector with the piezometric head in meters.

**Note**

The data were imported from the package **geoR**.

**Source**

Harper, W.V. and Furr, J.M. (1986) Geostatistical analysis of potentiometric data in the Wolfcamp Aquifer of the Palo Duro Basin, Texas. *Technical Report BMI/ONWI-587, Bettelle Memorial Institute, Columbus, OH.*

**References**

Cressie, N. A. C. (1993) *Statistics for Spatial Data*, Wiley, New York, [doi:10.1002/9781119115151](https://doi.org/10.1002/9781119115151).

Papritz, A. and Moyeed, R. (2001) Parameter uncertainty in spatial prediction: checking its importance by cross-validating the Wolfcamp and Rongelap data sets, *GeoENV 2000: Geostatistical for Environmental Applications*. Eds P. Monestiez, D. Allard, R. Froidevaux. Kluwer, [doi:10.1007/9789401008105](https://doi.org/10.1007/9789401008105).

**Examples**

```
data(wolfcamp)
summary(wolfcamp)
```

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