

Package ‘regress’

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Title Gaussian linear models with linear covariance structure

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Description Functions to fit Gaussian linear model by maximising the residual log likelihood where the covariance structure can be written as a linear combination of known matrices. Can be used for multivariate models and random effects models. Easy straight forward manner to specify random effects models, including random interactions. Code now optimised to use Sherman Morrison Woodbury identities for matrix inversion in random effects models. We’ve added the ability to fit models using any kernel as well as a function to return the mean and covariance of random effects conditional on the data (BLUPs).

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URL <http://www.csiro.au>

Suggests nlme, MASS

SystemRequirements

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*Fit a Gaussian Linear Model with Linear Covariance Structure***Description**

Fits Gaussian linear models in which the covariance structure can be expressed as a linear combination of known matrices. For example, block effects models and spatial models that include a nugget effect. Fits model by maximising the residual log likelihood, also known as the REML log likelihood or restricted log likelihood. Uses a Newton-Raphson algorithm to maximise the residual log likelihood. Some computational efficiencies are achieved when all variance components are associated with factors. In such a random effects model the matrix inversion is computed using the Sherman Morrison Woodbury identities.

Usage

```
regress(formula, Vformula, identity=TRUE, kernel=NULL,
        start=NULL, taper=NULL, pos, verbose=0, gamVals=NULL,
        maxcyc=50, tol=1e-4, data,
        fraction=NULL, print.level=NULL)
```

Usage

```
regress(formula, Vformula, identity=TRUE, kernel=NULL,
        start=NULL, taper=NULL, pos, verbose=0, gamVals=NULL,
        maxcyc=50, tol=1e-4, data,
        fraction=NULL, print.level=NULL)
```

Arguments

formula	a symbolic description of the model to be fitted. The details of model specification are the same as for <code>lm</code>
Vformula	Specifies the matrices to include in the covariance structure. Each term is either a symmetric matrix, or a factor. Independent Gaussian random effects are included by passing the corresponding block factor.
identity	Logical variable, includes the identity as the final matrix of the covariance structure. Default is TRUE
kernel	Compute the log likelihood based on a reduced observation TY where T has this kernel. Default value of NULL assumes that the kernel matches the fixed effects model matrix X corresponding to REML. Setting <code>kernel=0</code> gives the ordinary likelihood and <code>kernel=1</code> gives the one dimensional subspace of constant vectors.
start	Specify the variance components at which the Newton-Raphson algorithm starts. Default value is <code>rep(var(y), k)</code> .
taper	The proportion of each step to take. A vector of values from 0 to 1 of length <code>maxcyc</code> . Default value takes smaller steps initially.

pos	logical vector of length k, where k is the number of matrices in the covariance structure. Indicates which variance components are positive (TRUE) and which are real (FALSE). Important for multivariate problems.
verbose	Controls level of time output, takes values 0, 1 or 2, Default is 0, level 1 gives parameter estimates and value of log likelihood at each stage.
gamVals	When k=2, the marginal log likelihood based on the residual configuration statistic (see Tunnicliffe Wilson(1989)), is evaluated first at $(1-\text{gam}) V1 + \text{gam} V2$ for each value of gam in gamVals, a set of values from the unit interval. Subsequently the Newton-Raphson algorithm is started at variance components corresponding the the value of gam that has the highest marginal log likelihood. This is overridden if start is specified.
maxcyc	Maximum number of cycles allowed. Default value is 50. A warning is output to the screen if this is reached before convergence.
tol	Convergence criteria. If the change in residual log likelihood for one cycle is less than tol the algorithm finishes. Default value is $1e-4$.
data	an optional data frame containing the variables in the model. By default the variables are taken from 'environment(formula)', typically the environment from which 'regress' is called.
fraction	Deprecated, see taper
print.level	Deprecated

Details

As the code is running it outputs the variance components, and the residual log likelihood at each iteration.

To avoid confusion over terminology. I define variance components to be the multipliers of the matrices and variance parameters to the parameter space over which the Newton-Raphson algorithm is run. I can force a component to be positive be defining the corresponding variance parameter on the log scale.

All output to the screen is for variance components (i.e. the multiples of the matrices). Values for start are on the variance component scale. Use pos to force certain variance components to be positive.

NOTE: The final stage of the algorithm converts the estimates of the variance components and the Fisher Information to the usual linear scale, i.e. as if pos were a vector of zeroes.

NOTE: No predict functionality is provided with regress due to some ambiguity. Are we predicting conditional on the observed data. Are we predicting observations from the fitted model itself? It is all normal anyway so it is straightforward, see our paper on regress.

When you fit a Gaussian regression model using `fit <- regress(y~X, ~V, kernel=K)` the function computes the log likelihood based on the reduced observation $TY \sim N(TX, T V T')$, where T is a linear transformation with kernel K . Only $n-k$ degrees of freedom are available. Ordinary likelihood corresponds to $K=0$, and REML to $K=X$, but these are not the only options.

When you fit two nested Gaussian models ($X0$ subset of $X1$ and $V0$ subset of $V1$) using the commands:

```
fit0 <- regress(y~X0, ~V0, kernel=K)
```

```
fit1 <- regress(y~X1, ~V1, kernel=K)
```

then the likelihood ratio statistic $\text{fit1}\$lik - \text{fit0}\lik is the ordinary likelihood ratio based on the Gaussian observation TY where the kernel of T is K . So if you set $\text{kernel}=0$, you get the ordinary likelihood ratio based on the complete observation y ; And if you set $\text{kernel}=1$, you get the likelihood ratio based on simple contrasts $y_i - y_j$ only. So in the latter case, you have only $n-1$ degrees of freedom to work with. And if you set $\text{kernel}=X0$, you get the likelihood ratio based on contrasts Ty with kernel $X0$, which for fit0 is the REML likelihood.

Value

trace	Matrix with one row for each iteration of algorithm. Each row contains the residual log likelihood, marginal log likelihood, variance parameters and increments.
llik	Value of the marginal log likelihood at the point of convergence.
cycle	Number of cycles to convergence.
rdf	Residual degrees of freedom.
beta	Estimate of the linear effects.
beta.cov	Estimate of the covariance structure for terms in beta.
beta.se	Standard errors for terms in beta.
sigma	Variance component estimates, interpretation does not depend on value of pos
sigma.cov	Covariance matrix for the variance component estimates based on the Fisher Information at the point of convergence.
W	Inverse of covariance matrix at point of convergence.
Q	$I - X^T (X^T W X)^{-1} X^T W$ at point of convergence.
fitted	$X \text{beta}$, the fitted values.
predicted	If $\text{identity}=\text{TRUE}$, decompose y into the part associated with the identity and that associated with the rest of the variance structure, this second part is the predicted values. If $\Sigma = V1 + V2$ at point of convergence then $y = V1 W y + V2 W y$ is the decomposition.
pos	Indicator for the scale for each variance parameter.
Vnames	Names associated with each variance component, used in <code>print.regress</code> .
formula	Copy of formula
Vformula	Updated version of <code>Vformula</code> to include identity if necessary
Kcolnames	Names associated with the kernel
model	Response, covariates and matrices/factors to be used for model fitting
Z	Design matrices associated with the random effects, used for computation of BLUPs

Author(s)

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References

G. Tunncliffe Wilson (1989), "On the use of marginal likelihood in time series model estimation." *JRSS B*, Vol 51, No 1, 15-27.

D. Clifford and P. McCullagh (2006), "The regress function" *R News* 6(2):6-10

Weisstein, Eric W. "Woodbury Formula." From MathWorld—A Wolfram Web Resource. <http://mathworld.wolfram.com/WoodburyFormula.html>

Weisstein, Eric W. "Sherman-Morrison Formula." From MathWorld—A Wolfram Web Resource. <http://mathworld.wolfram.com/Sherman-MorrisonFormula.html>

Examples

```
#####
## Comparison with lme
#####

## Example of Random Effects model from Venables and Ripley, page 205
library("nlme")
library("regress")

citation("regress")

names(Oats) <- c("B", "V", "N", "Y")
Oats$N <- as.factor(Oats$N)

## Using regress
oats.reg <- regress(Y~N+V, ~B+I(B:V), identity=TRUE, verbose=1, data=Oats)
summary(oats.reg)

## Using lme
oats.lme <- lme(Y~N+V, random=~1|B/V, data=Oats, method="REML")
summary(oats.lme)

## print and summary
oats.reg
print(oats.reg)
summary(oats.reg)

ranef(oats.lme)
BLUP(oats.reg)

rm(oats.reg, oats.lme, Oats)

#####
## Computation of BLUPs
#####

ex2 <- list()
ex2 <- within(ex2, {

  ## Set up example
  set.seed(1001)
```

```

n <- 101
x1 <- runif(n)
x2 <- seq(0,1,l=n)
z1 <- gl(4,10,n)
z2 <- gl(6,1,n)

X <- model.matrix(~1 + x1 + x2)
Z1 <- model.matrix(~z1-1)
Z2 <- model.matrix(~z2-1)

## Create the individual random and fixed effects
beta <- c(1,2,3)
eta1 <- rnorm(ncol(Z1),0,10)
eta2 <- rnorm(ncol(Z2),0,10)
eps <- rnorm(n,0,3)

## Combine them into a response
y <- X %*% beta + Z1 %*% eta1 + Z2 %*% eta2 + eps
})

## Data frame containing all we need for model fitting
regressDF <- with(ex2,data.frame(y,x1,x2,z1,z2))
rm(ex2)

## Fit the model using regress
regress.output <- regress(y~1 + x1 + x2,~z1 + z2,data=regressDF)

summary(regress.output)

blup1 <- BLUP(regress.output,RE="z1")
blup1$Mean
blup1$Variance
blup1$Covariance
cov2cor(blup1$Covariance) ## Large correlation terms

blup2 <- BLUP(regress.output) ## Joint BLUP of z1 and z2 by default
blup2$Mean
blup2$Variance
cov2cor(blup2$Covariance) ## Strong negative correlation between BLUPs
## for z1 and z2

rm(blup1,blup2)

#####
## Examples of use of kernel
#####

## LRT for z2 using ordinary likelihood
with(regressDF,{
  K <- 0
  model1 <- regress(y~1+x1,~z1,kernel=K)
  model2 <- regress(y~1+x1+x2,~z1,kernel=K)
  2*(model2$llik - model1$llik)
}

```

```
})

## REML LRT for z2
with(regressDF,{
  K <- model.matrix(~1+x1+x2)
  model1 <- regress(y~1+x1,~z1,kernel=K)
  model2 <- regress(y~1+x1+x2,~z1,kernel=K)
  2*(model2$l1ik - model1$l1ik)
})

## LRT for x2 based on a reduced observation TY with kernel K
with(regressDF,{
  K <- model.matrix(~1+x1)
  model1 <- regress(y~1+x1,~z1,kernel=K)
  model2 <- regress(y~1+x1+x2,~z1,kernel=K)
  2*(model2$l1ik - model1$l1ik)
})

rm(regressDF, regress.output)
```

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