

Package ‘regress’

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Title Gaussian linear models with linear covariance structure

Author David Clifford and Peter McCullagh. Additional contributions by HJ Auinger.

Maintainer David Clifford <david.clifford@csiro.au>

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)
```

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 <code>k</code> , where <code>k</code> 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 <code>k=2</code> , the marginal log likelihood based on the residual configuration statistic (see Tunnicliffe Wilson(1989)), is evaluated first at $(1 - \text{gam}) V_1 + \text{gam} V_2$ |

| | |
|--------------------------|--|
| | for each value of <code>gam</code> in <code>gamVals</code> , a set of values from the unit interval. Subsequently the Newton-Raphson algorithm is started at variance components corresponding to the value of <code>gam</code> that has the highest marginal log likelihood. This is overridden if <code>start</code> is specified. |
| <code>maxcyc</code> | Maximum number of cycles allowed. Default value is 50. A warning is output to the screen if this is reached before convergence. |
| <code>tol</code> | Convergence criteria. If the change in residual log likelihood for one cycle is less than <code>tol</code> the algorithm finishes. Default value is $1e-4$. |
| <code>data</code> | an optional data frame containing the variables in the model. By default the variables are taken from <code>'environment(formula)'</code> , typically the environment from which <code>'regress'</code> is called. |
| <code>fraction</code> | Deprecated, see <code>taper</code> |
| <code>print.level</code> | 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 by 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 `fit1$loglik - fit0$loglik` is the ordinary likelihood ratio based on the Gaussian observation TY where the kernel of T is K . So if you set `kernel=0`, you get the ordinary likelihood ratio based on the complete observation y ; And if you set `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 `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 | $X \beta$, the fitted values. |
| predicted | If identity=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. This is the conditional expectation for new observations conditional on the observed data. |
| predictedVariance | Variance of new observations conditional on the observed data |
| predictedVariance2 | Additional variance associated with the uncertainty of beta. Can be added to predictedVariance |
| pos | Indicator for the scale for each variance parameter. |
| Vnames | Names associated with each variance component, used in print.regress. |
| formula | Copy of formula |
| Vformula | Updated version of Vformula 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)

David Clifford, Peter McCullagh

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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