

R function solve fails for tree with large condition number

We report two equivalent cases where the tree fails to return the inverse through `solve`:

Case 1: the tree with tiny tip

```
MakeTree <- function(x) {
  return(ape::read.tree(text=paste0("(A:",x,"B:",x,"):5,C:",5+x,");
  "")))
}
traits <- c(A=0,B=0,C=1)
x.vals <- 10^(seq(from=-14, to=-16, by=-0.2))
solve.return <- rep(NA, length(x.vals))
continuous.lnl <- rep(NA, length(x.vals))
continuous.sigsq <- rep(NA, length(x.vals))
kappa.return <- rep(NA, length(x.vals))
for (i in seq_along(x.vals)) {
  phy <- MakeTree(x.vals[i])
  try(solve.return[i] <- solve(ape::vcv(phy))[1,1]) # If work, it returns c11 in C.
  try(kappa.return[i] <- kappa(ape::vcv(phy)))
  try(continuous.lnl[i] <- geiger::fitContinuous(phy, traits, model="BM")$opt$lnL)
  try(continuous.sigsq[i] <- geiger::fitContinuous(phy, traits, model="BM")$opt$sigsq)
}

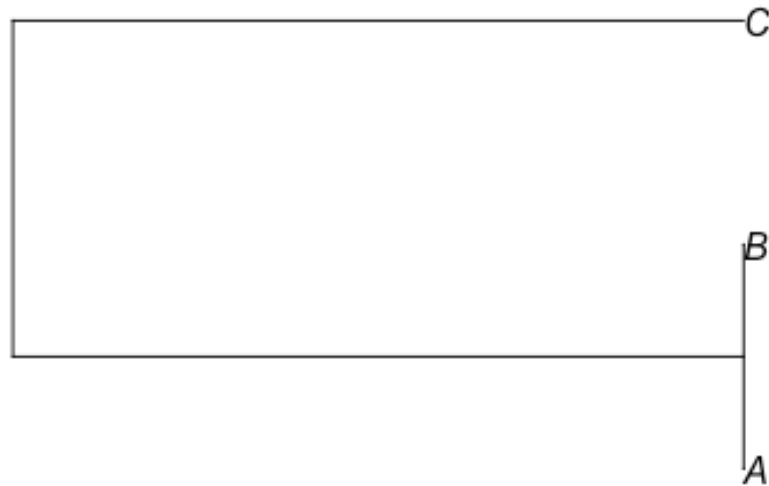
## Registered S3 method overwritten by 'geiger':
##   method      from
##   unique.multiPhylo ape

## Error in solve.default(ape::vcv(phy)) :
##   系統計算上是獨特的: 互反條件數=1.59872e-16
## Error in solve.default(ape::vcv(phy)) :
##   系統計算上是獨特的: 互反條件數=1.59872e-16
## Error in solve.default(ape::vcv(phy)) :
##   Lapack routine dgesv: system is exactly singular: U[2,2] = 0
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##   Lapack routine dgesv: system is exactly singular: U[2,2] = 0
```

```
cbind(x.vals, solve.return, kappa.return, continuous.lnl, continuous.sigsq)
```

```
##           x.vals solve.return kappa.return continuous.lnl
## [1,] 1.000000e-14 5.117727e+13 9.951643e+14      15.00706
## [2,] 6.309573e-15 8.042142e+13 1.592263e+15      15.23732
## [3,] 3.981072e-15 1.407375e+14 3.184526e+15      15.46758
## [4,] 2.511886e-15 2.251800e+14 3.980657e+15      15.69784
## [5,] 1.584893e-15 2.814750e+14 3.980657e+15      15.92810
## [6,] 1.000000e-15           NA 7.961315e+15      16.15836
## [7,] 6.309573e-16           NA 7.961315e+15      16.38862
## [8,] 3.981072e-16           NA           Inf      16.61887
## [9,] 2.511886e-16           NA           Inf      16.84913
## [10,] 1.584893e-16           NA           Inf      17.07939
## [11,] 1.000000e-16           NA           Inf      17.30965
##           continuous.sigsq
## [1,]           0.03333333
## [2,]           0.03333333
## [3,]           0.03333333
## [4,]           0.03333333
## [5,]           0.03333333
## [6,]           0.03333333
## [7,]           0.03333333
## [8,]           0.03333333
## [9,]           0.03333333
## [10,]          0.03333333
## [11,]          0.03333333
```

```
plot(phy)
```



As it shows that when tip has length less than 10^{-15} , the solve method fails to return the inverse of the variance covariance matrix C .

Case 2: Extremely long time since the root to the most common ancestor for all tips

```
library(TreeSim)

## Loading required package: ape

## Loading required package: geiger

treesize<-10
age.array<-10^(seq(from=14, to=16, length.out=10))

solve.return <- rep(NA, length(age.array))
continuous.lnl <- rep(NA, length(age.array))
continuous.sigsq <- rep(NA, length(age.array))
kappa.return <- rep(NA, length(age.array))

for(ageIndex in 1:length(age.array)){
  age<-age.array[ageIndex]
  tree<-sim.bd.taxa.age(n=treesize,numbsim=1,lambda=0.5,mu=0.1,age=age,
mrca=TRUE)[[1]]
```

```

traits<-c(1,1,1,1,1,0,0,0,0,0)
names(traits)<-tree$tip.label
print(kappa(vcv(tree)))
try(solve.return[ageIndex] <- solve(ape::vcv(tree))[1,1])
try(kappa.return[ageIndex] <- kappa(ape::vcv(tree)))
try(continuous.lnl[ageIndex] <- geiger::fitContinuous(tree, traits, model="BM")$opt$lnL)
try(continuous.sigsq[ageIndex] <- geiger::fitContinuous(tree, traits, model="BM")$opt$sigsq)
}

## [1] 4.8459e+15
## [1] 1.544379e+15
## [1] 2.657303e+16
## Error in solve.default(ape::vcv(tree)) :
## 系統計算上是獨特的：互反條件數=3.27921e-17
## [1] 3.159116e+15
## Error in solve.default(ape::vcv(tree)) :
## 系統計算上是獨特的：互反條件數=2.16834e-16
## [1] 7.547765e+15
## Error in solve.default(ape::vcv(tree)) :
## 系統計算上是獨特的：互反條件數=1.00009e-16
## [1] 3.523674e+15
## Error in solve.default(ape::vcv(tree)) :
## 系統計算上是獨特的：互反條件數=1.44059e-16
## [1] 6.005703e+15
## Error in solve.default(ape::vcv(tree)) :
## 系統計算上是獨特的：互反條件數=1.00295e-16
## [1] 8.204332e+15
## Error in solve.default(ape::vcv(tree)) :
## 系統計算上是獨特的：互反條件數=6.0078e-17
## [1] 1.835383e+16
## Error in solve.default(ape::vcv(tree)) :
## 系統計算上是獨特的：互反條件數=2.2313e-17
## [1] 1.344292e+34
## Error in solve.default(ape::vcv(tree)) :
## Lapack routine dgesv: system is exactly singular: U[6,6] = 0

cbind(age.array, solve.return, kappa.return, continuous.lnl, continuous.sigsq)

##          age.array solve.return kappa.return continuous.lnl
## [1,] 1.000000e+14    0.2831858 4.845900e+15 -3.772645e+01
## [2,] 1.668101e+14    0.2759097 1.544379e+15  1.274904e+02
## [3,] 2.782559e+14          NA 2.657303e+16 -4.397268e+01
## [4,] 4.641589e+14          NA 3.159116e+15 -3.965892e+01
## [5,] 7.742637e+14          NA 7.547765e+15 -3.523881e+01
## [6,] 1.291550e+15          NA 3.523674e+15 -3.799792e+01
## [7,] 2.154435e+15          NA 6.005703e+15 -3.696301e+01
## [8,] 3.593814e+15          NA 8.204332e+15 -3.596696e+01

```

```
## [9,] 5.994843e+15      NA 1.835383e+16 -4.382316e+01
## [10,] 1.000000e+16     NA 1.344292e+34 -1.000000e+200
##      continuous.sigsq
## [1,] 1.262739e-01
## [2,] 2.997421e-16
## [3,] 4.839934e-01
## [4,] 8.617201e-02
## [5,] 4.588867e-02
## [6,] 3.091589e-02
## [7,] 2.225554e-02
## [8,] 1.798607e-02
## [9,] 1.153720e-01
## [10,] 2.688110e+43

plot(tree)
```



As it shows that when the age since the root to the most recent common ancestor is greater than 10^{14} , the solve method fails to return the inverse of the variance covariance matrix C .