randomForest

Random Forest Tests

Here I am playing around with Random Forest Classification in a data set I make up.

The data set

First, I am setting up the session and the data set. I am essentially imagining a sample of individuals, for whom we know age, weight, an affected trait, maybe fitness (V02max), and have genotyped (0/1/2) four loci. We also have the phenotype of interest, perhaps a disease (0/1) that affects fitness (age and weight do, too), and is in turn caused by three of the four genotyped loci. I wanted to see how a random forest would deal with this scenario.

```
library(tidyverse)
```

```
-- Attaching core tidyverse packages ------------------------ tidyverse 2.0.0 --
v dplyr     1.1.1     v readr     2.1.4
v forcats   1.0.0     v stringr   1.5.0
v ggplot2   3.4.1     v tibble    3.2.1
v lubridate 1.9.2     v tidyr     1.3.0
v purrr     1.0.1
-- Conflicts ------------------------------------------ tidyverse_conflicts() --
x dplyr::filter() masks stats::filter()
x dplyr::lag()    masks stats::lag()
i Use the conflicted package (<http://conflicted.r-lib.org/>) to force all conflicts to becom
```

```
library(randomForest)
```

```
randomForest 4.7-1.1
Type rfNews() to see new features/changes/bug fixes.

Attaching package: 'randomForest'

The following object is masked from 'package:dplyr':

    combine

The following object is masked from 'package:ggplot2':

    margin
```

```r
count_individuals = 2000
count_loci = 4

genotype_matrix <-
  matrix(
    rbinom(count_individuals * count_loci, 1, 0.5) + rbinom(count_individuals * count_loci
    nrow = count_individuals,
    ncol = count_loci
  )
genotype_df <- as_tibble(genotype_matrix)
```

```
Warning: The `x` argument of `as_tibble.matrix()` must have unique column names if
`.name_repair` is omitted as of tibble 2.0.0.
i Using compatibility `.name_repair`.
```

```r
colnames(genotype_df) <- paste0("locus_", 1:count_loci)

additional_data <-
  tibble(
    ID = 1:count_individuals,
    weight = rnorm(count_individuals, mean = 80, sd = 5),
    age = sample(20:80, count_individuals, replace = TRUE)
  )

data_combined <- bind_cols(additional_data, genotype_df)
```

```r
make_binary_trait = function(row) {
  # here are the rules how the binary trait is generated
  data_combined_slice <- slice(data_combined, row)
  #print(data_combined_slice)
  individual_risk <- 0
  individual_risk <-
    individual_risk + (pull(data_combined_slice, locus_1)) * 0.1 # additive effect
  individual_risk <-
    individual_risk + (pull(data_combined_slice, locus_2)) * 0.1
  individual_risk <-
    individual_risk + (pull(data_combined_slice, locus_3)) * 0.1
  individual_risk <-
    individual_risk + ((pull(data_combined_slice, locus_1) == 2) * (pull(data_combined_sli
                                                                      2)) * 0.4

  individual_risk <-
    individual_risk + ((pull(data_combined_slice, locus_1) == 2) * (pull(data_combined_sli
                                                                      2) * (pull(data_comb
  if (individual_risk > 1) {
    individual_risk <- 1
  }
  phenotype <- rbinom(1, 1, individual_risk)
  return(phenotype)
}

add_affected_trait <- function(row) {
  data_combined_slice <- slice(data_combined, row)
  mean <-
    40 # the average in the healthy population of a trait, say VO2max
  mean <-
    mean - (pull(data_combined_slice, phenotype) == 1) * 5 # decrease in 5 for those with
  mean <- mean - pull(data_combined_slice, weight) * 0.1 # decrease with weight
  mean <- mean - pull(data_combined_slice, age) * 0.1 # decrease with age
  return(rnorm(1, mean, sd = 3))
}

# add the phenotype and affected trait to the data frame

data_combined$phenotype <-
  as.factor(unlist(lapply(
    1:nrow(data_combined), make_binary_trait
  )))
```

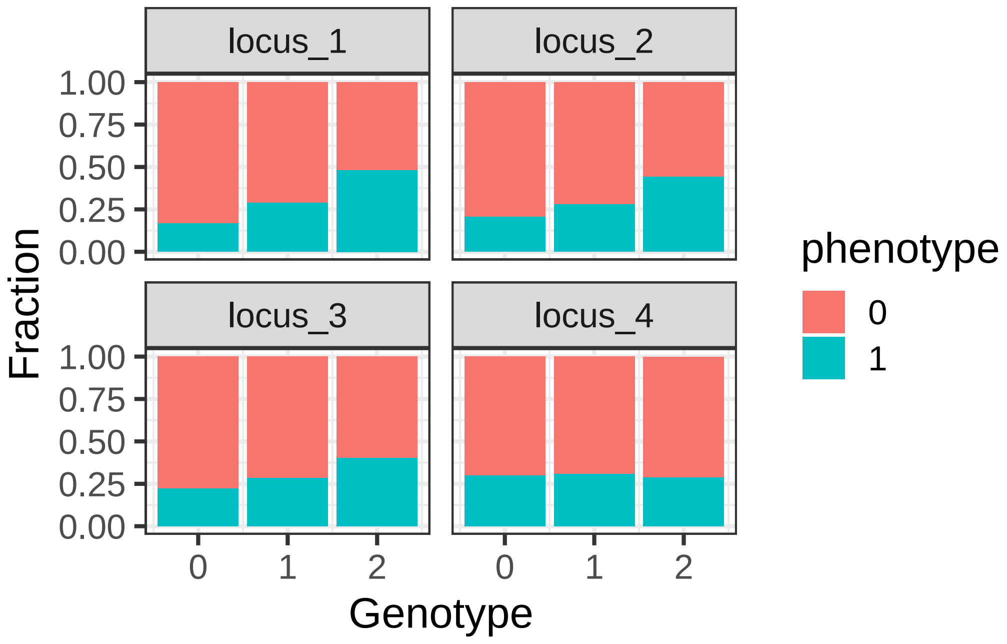
```
data_combined$affected_trait <-
  unlist(lapply(1:nrow(data_combined), add_affected_trait))
data_combined$weight = as.numeric(scale(data_combined$weight, center = TRUE, scale =
                                          TRUE))
data_combined$age = as.numeric(scale(data_combined$age, center = TRUE, scale =
                                       TRUE))
data_combined$affected_trait = as.numeric(scale(
  data_combined$affected_trait,
  center = TRUE,
  scale = TRUE
))

summary(data_combined$phenotype)
```

```
   0    1
1398  602
```

Above, you can see the distribution of the phenotype. A bit imbalanced, but still plenty of samples.

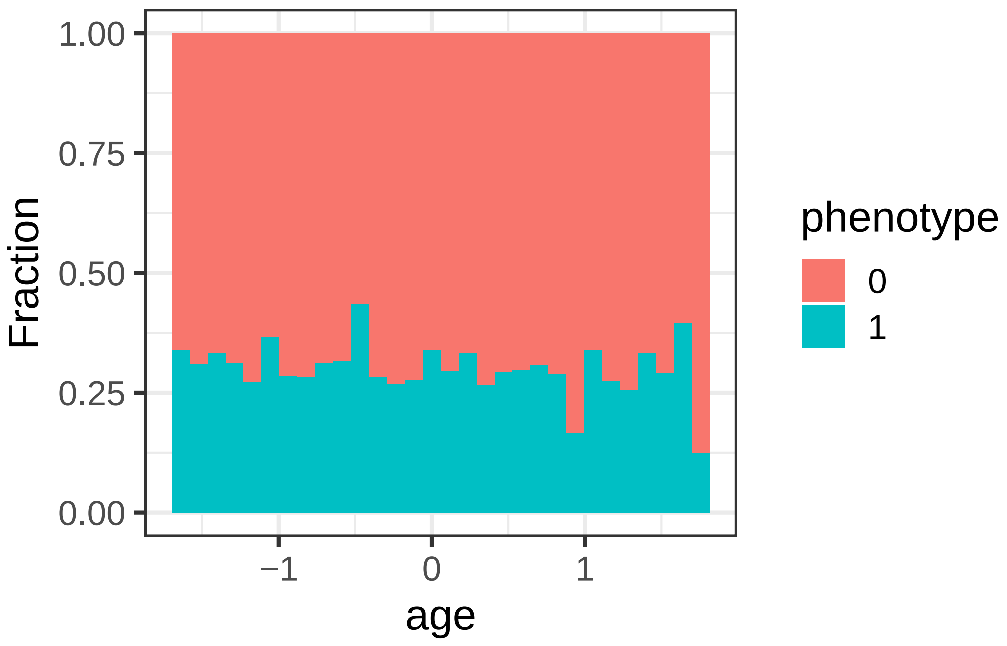
Let's have a look at the traits we have. **But note that they have ben scaled for better modelling.**

```
library(ggplot2)
ggplot(data_combined%>%pivot_longer(cols=c(locus_1,locus_2,locus_3,locus_4)), aes(value, g
    geom_bar(position="fill")+facet_wrap(~name)+xlab("Genotype")+ylab("Fraction")+theme_bw
```



```
ggplot(data_combined, aes(age, fill = phenotype)) +
  geom_histogram(position = "fill")+theme_bw(16)+ylab("Fraction")
```

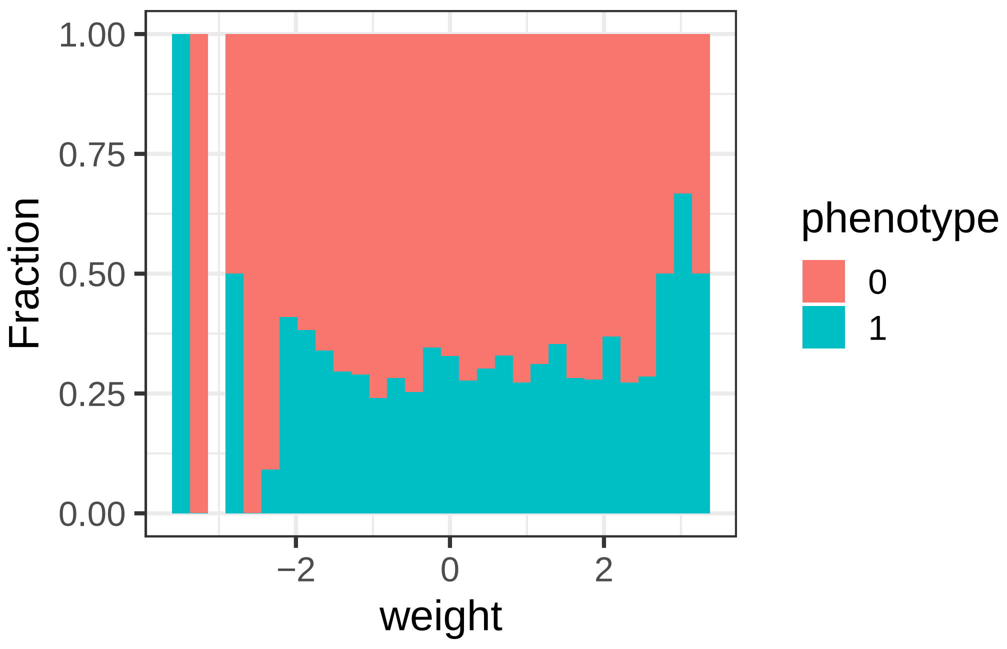
```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



```r
ggplot(data_combined, aes(weight, fill = phenotype)) +
  geom_histogram(position = "fill")+theme_bw(16)+ylab("Fraction")
```

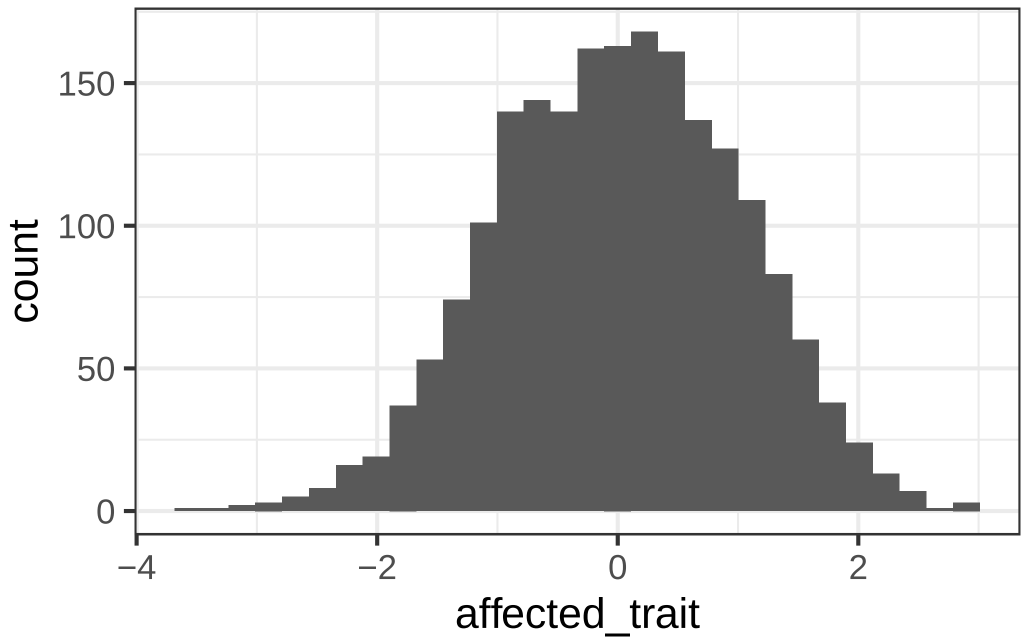
```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

```
Warning: Removed 2 rows containing missing values (`geom_bar()`).
```



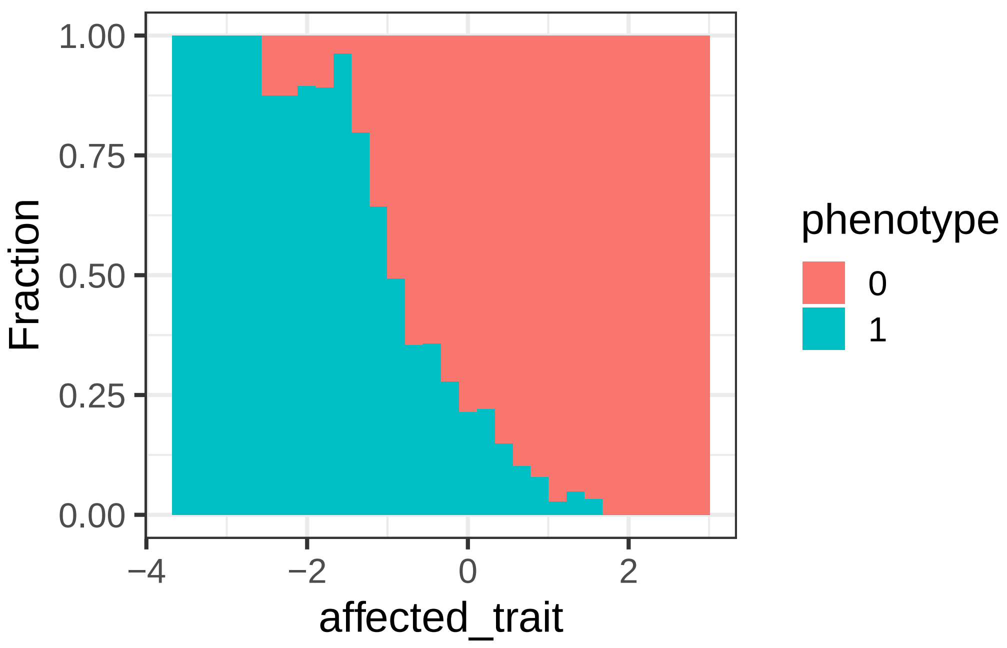
```r
ggplot(data_combined, aes(affected_trait)) +
  geom_histogram()+theme_bw(16)
```

```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

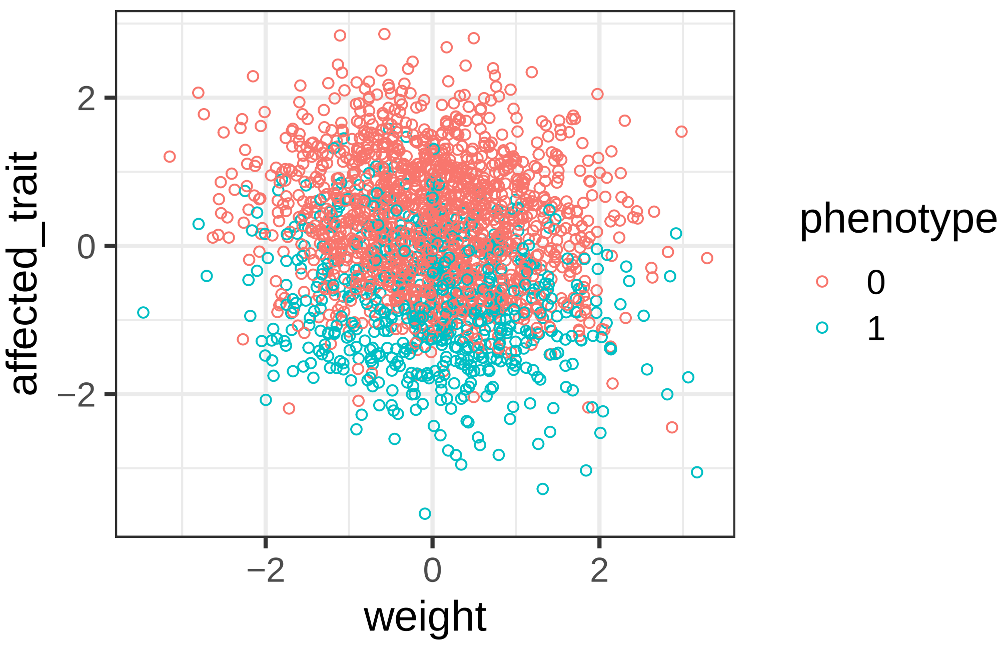


```r
ggplot(data_combined, aes(affected_trait, fill = phenotype)) +
  geom_histogram(position = "fill")+theme_bw(16)+ylab("Fraction")
```

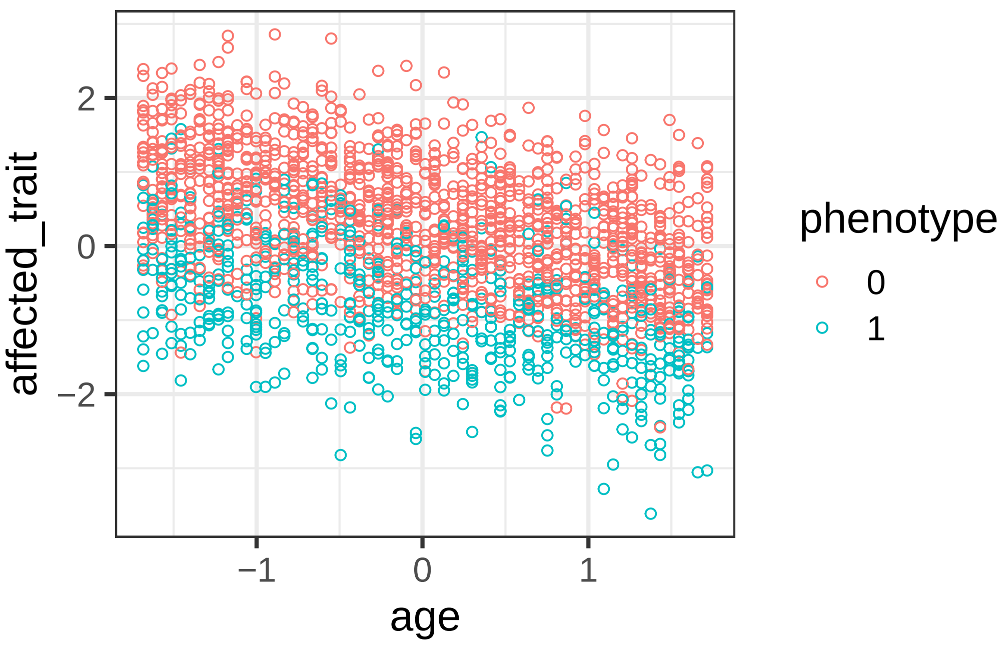
```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



```r
ggplot(data_combined, aes(weight, affected_trait, color = phenotype)) +
  geom_point(shape = 1)+theme_bw(16)
```



```
ggplot(data_combined, aes(age, affected_trait, color = phenotype)) +
  geom_point(shape = 1)+theme_bw(16)
```

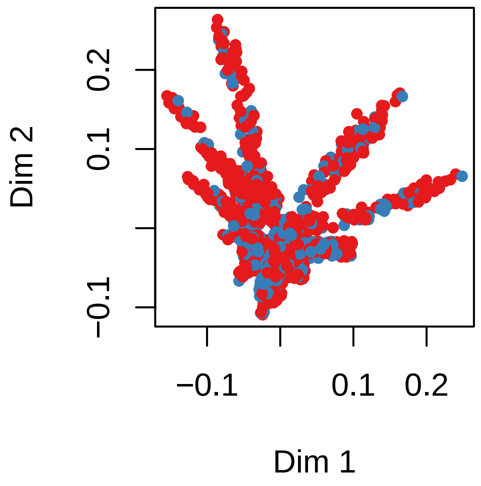


OK, definitely realistic looking and tons of noise!

I will first see if an unsupervised forest finds some relevant structure in the data.

```r
data_combined.urf <-
  randomForest(select(data_combined,-1,-(ncol(data_combined) - 1)), ntree =
                   count_individuals * 10)
MDSplot(data_combined.urf, data_combined$phenotype)
```

```
Warning in RColorBrewer::brewer.pal(nlevs, "Set1"): minimal value for n is 3, returning reque
```



Without any supervision, we do not see strong structuring along the phenotype (color), but some can be seen.

Can we get a good prediction with a random forest classification after some tuning?

```r
library(caret)
```

```
Loading required package: lattice


Attaching package: 'caret'

The following object is masked from 'package:purrr':

    lift
```

```r
# split the data
ids <- createDataPartition(data_combined$phenotype, p = 0.8, list = F)
train_set <- data_combined[ids, ]
test_set <- data_combined[-ids, ]

cn <- trainControl(method = "cv", number = 10)

grid <- expand.grid(mtry = 2:(ncol(train_set) - 1))

fit <-
  train(
    phenotype ~ .,
    data = train_set,

    method = "rf",
    trControl = cn,
    tuneGrid = grid,
    ntree = count_individuals * 10,
    maxnodes = 500
  )
```

Let's see how well the model works!

```r
p <- predict(fit, test_set %>% select(-(ncol(test_set) - 1)))

print(cM<-confusionMatrix(p, test_set$phenotype))
```

```
Confusion Matrix and Statistics

          Reference
Prediction   0   1
         0 261  49
         1  18  71

               Accuracy : 0.8321
                 95% CI : (0.7917, 0.8674)
    No Information Rate : 0.6992
    P-Value [Acc > NIR] : 7.523e-10

                  Kappa : 0.569
```

```
 Mcnemar's Test P-Value : 0.0002473

            Sensitivity : 0.9355
            Specificity : 0.5917
         Pos Pred Value : 0.8419
         Neg Pred Value : 0.7978
             Prevalence : 0.6992
         Detection Rate : 0.6541
   Detection Prevalence : 0.7769
      Balanced Accuracy : 0.7636

       'Positive' Class : 0
```

So, concluding for now, we have built a random forest that is a able find 93.55% of individuals with an imaginary disease that decreases their physical fitness and is determined by three loci in a additive and epistatic fashion. We would probably not be able to use this model on a large number of loci because of performance, but I am curious how well it still works when there are more loci (of course, building a new forest with those first).