Translucent box

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Setup

```
# General
library(dplyr)
```

```
##
## Attaching package: 'dplyr'
```

```
## The following objects are masked from 'package:stats':
##
##     filter, lag
```

```
## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```
library(ggplot2)
library(doParallel)
```

```
## Loading required package: foreach
```

```
## Loading required package: iterators
```

```
## Loading required package: parallel
```

```
# Modelling libraries
library(caret)
```

```
## Loading required package: lattice
```

```
library(lime)
```

```
##
## Attaching package: 'lime'
```

```
## The following object is masked from 'package:dplyr':
##
##     explain
```

```
library(pdp)
library(ICEbox)
```

```
## Loading required package: sfsmisc
```

```
##
## Attaching package: 'sfsmisc'
```

```
## The following object is masked from 'package:dplyr':
##
##     last
```

```
library(iml)
library(elasticnet)
```

```
## Loading required package: lars
```

```
## Loaded lars 1.2
```

```
library(INLA)
```

```
## Loading required package: Matrix
```

```
## Loading required package: sp
```

```
## This is INLA_19.09.03 built 2019-09-03 09:07:31 UTC.
## See www.r-inla.org/contact-us for how to get help.
## To enable PARDISO sparse library; see inla.pardiso()
```

```
library(palettetown)


# Phylogenetic libraries.
library(ape)
library(caper)
```

```
## Loading required package: MASS
```

```
##
## Attaching package: 'MASS'
```

```
## The following object is masked from 'package:dplyr':
##
##     select
```

```
## Loading required package: mvtnorm
```

```
source('helpers.R')

set.seed(100)
```

The data

First we need to read in the data.

```
p <- read.table(file = 'http://esapubs.org/archive/ecol/E090/184/PanTHERIA_1-0_WR05_Aug2008.txt',
  header = TRUE, sep = "\t", na.strings = c("-999", "-999.00"))


names(p)
```

```
##  [1] "MSW05_Order"                   "MSW05_Family"                  "MSW05_Genus"                   "MSW05
##  [6] "X1.1_ActivityCycle"            "X5.1_AdultBodyMass_g"          "X8.1_AdultForearmLen_mm"       "X13.1
## [11] "X3.1_AgeatFirstBirth_d"        "X18.1_BasalMetRate_mLO2hr"     "X5.2_BasalMetRateMass_g"       "X6.1_
## [16] "X9.1_GestationLen_d"           "X12.1_HabitatBreadth"          "X22.1_HomeRange_km2"           "X22.2
## [21] "X15.1_LitterSize"              "X16.1_LittersPerYear"          "X17.1_MaxLongevity_m"          "X5.3_
## [26] "X21.1_PopulationDensity_n.km2" "X10.1_PopulationGrpSize"       "X23.1_SexualMaturityAge_d"     "X10.2
## [31] "X12.2_Terrestriality"          "X6.2_TrophicLevel"             "X25.1_WeaningAge_d"            "X5.4_
## [36] "References"                    "X5.5_AdultBodyMass_g_EXT"      "X16.2_LittersPerYear_EXT"      "X5.6_
## [41] "X26.1_GR_Area_km2"             "X26.2_GR_MaxLat_dd"            "X26.3_GR_MinLat_dd"            "X26.4
## [46] "X26.6_GR_MinLong_dd"           "X26.7_GR_MidRangeLong_dd"      "X27.1_HuPopDen_Min_n.km2"      "X27.2
## [51] "X27.4_HuPopDen_Change"         "X28.1_Precip_Mean_mm"          "X28.2_Temp_Mean_01degC"        "X30.1
```

```
sapply(p, function(x) mean(is.na(x))) %>% sort
```

```
##                   MSW05_Order                   MSW05_Family                   MSW05_Genus                     M
##                     0.0000000                     0.0000000                     0.0000000
##            X26.2_GR_MaxLat_dd            X26.3_GR_MinLat_dd       X26.4_GR_MidRangeLat_dd          X26.5_G
##                     0.1381093                     0.1381093                     0.1381093
##      X27.1_HuPopDen_Min_n.km2     X27.2_HuPopDen_Mean_n.km2       X27.3_HuPopDen_5p_n.km2         X27.4_HuP
##                     0.1381093                     0.1381093                     0.1381093
##             X30.1_AET_Mean_mm             X30.2_PET_Mean_mm                    References          X5.1_Adu
##                     0.2051329                     0.2051329                     0.2307976
```

```
##             X15.1_LitterSize             X6.1_DietBreadth            X6.2_TrophicLevel     X13.1_AdultHe
##                    0.5382201                    0.6009970                    0.6009970
##           X25.1_WeaningAge_d       X5.3_NeonateBodyMass_g    X23.1_SexualMaturityAge_d          X17.1_Ma
##                    0.7850812                    0.7996677                    0.8059453
##          X16.1_LittersPerYear          X22.1_HomeRange_km2         X10.2_SocialGrpSize    X14.1_Interbir
##                    0.8349335                    0.8694609                    0.8694609
##     X18.1_BasalMetRate_mLO2hr       X5.2_BasalMetRateMass_g       X5.4_WeaningBodyMass_g        X2.1_Ageat
##                    0.8942024                    0.8942024                    0.9100812
##      X16.2_LittersPerYear_EXT      X10.1_PopulationGrpSize   X13.2_NeonateHeadBodyLen_mm          X7.1_Di
##                    0.9272526                    0.9283604                    0.9582718
##    X5.6_NeonateBodyMass_g_EXT
##                    0.9955687
```

```
sapply(p, class)
```

```
##                   MSW05_Order                  MSW05_Family                    MSW05_Genus                  M
##                      "factor"                      "factor"                       "factor"
##          X5.1_AdultBodyMass_g       X8.1_AdultForearmLen_mm     X13.1_AdultHeadBodyLen_mm        X2.1_Ageat
##                     "numeric"                     "numeric"                      "numeric"
##       X5.2_BasalMetRateMass_g             X6.1_DietBreadth          X7.1_DispersalAge_d          X9.1_Ge
##                     "numeric"                     "numeric"                      "numeric"
##     X22.2_HomeRange_Indiv_km2    X14.1_InterbirthInterval_d             X15.1_LitterSize         X16.1_Li
##                     "numeric"                     "numeric"                      "numeric"
##   X13.2_NeonateHeadBodyLen_mm X21.1_PopulationDensity_n.km2       X10.1_PopulationGrpSize     X23.1_SexualM
##                     "numeric"                     "numeric"                      "numeric"
##          X12.2_Terrestriality             X6.2_TrophicLevel           X25.1_WeaningAge_d        X5.4_Weani
##                     "numeric"                     "integer"                      "numeric"
##      X5.5_AdultBodyMass_g_EXT      X16.2_LittersPerYear_EXT    X5.6_NeonateBodyMass_g_EXT    X5.7_WeaningBo
##                     "numeric"                     "numeric"                      "numeric"
##            X26.3_GR_MinLat_dd       X26.4_GR_MidRangeLat_dd          X26.5_GR_MaxLong_dd          X26.6_G
##                     "numeric"                     "numeric"                      "numeric"
##     X27.2_HuPopDen_Mean_n.km2       X27.3_HuPopDen_5p_n.km2         X27.4_HuPopDen_Change          X28.1_Pr
##                     "numeric"                     "numeric"                      "numeric"
##             X30.2_PET_Mean_mm
##                     "numeric"
```

```
dim(p)
```

```
## [1] 5416   55
```

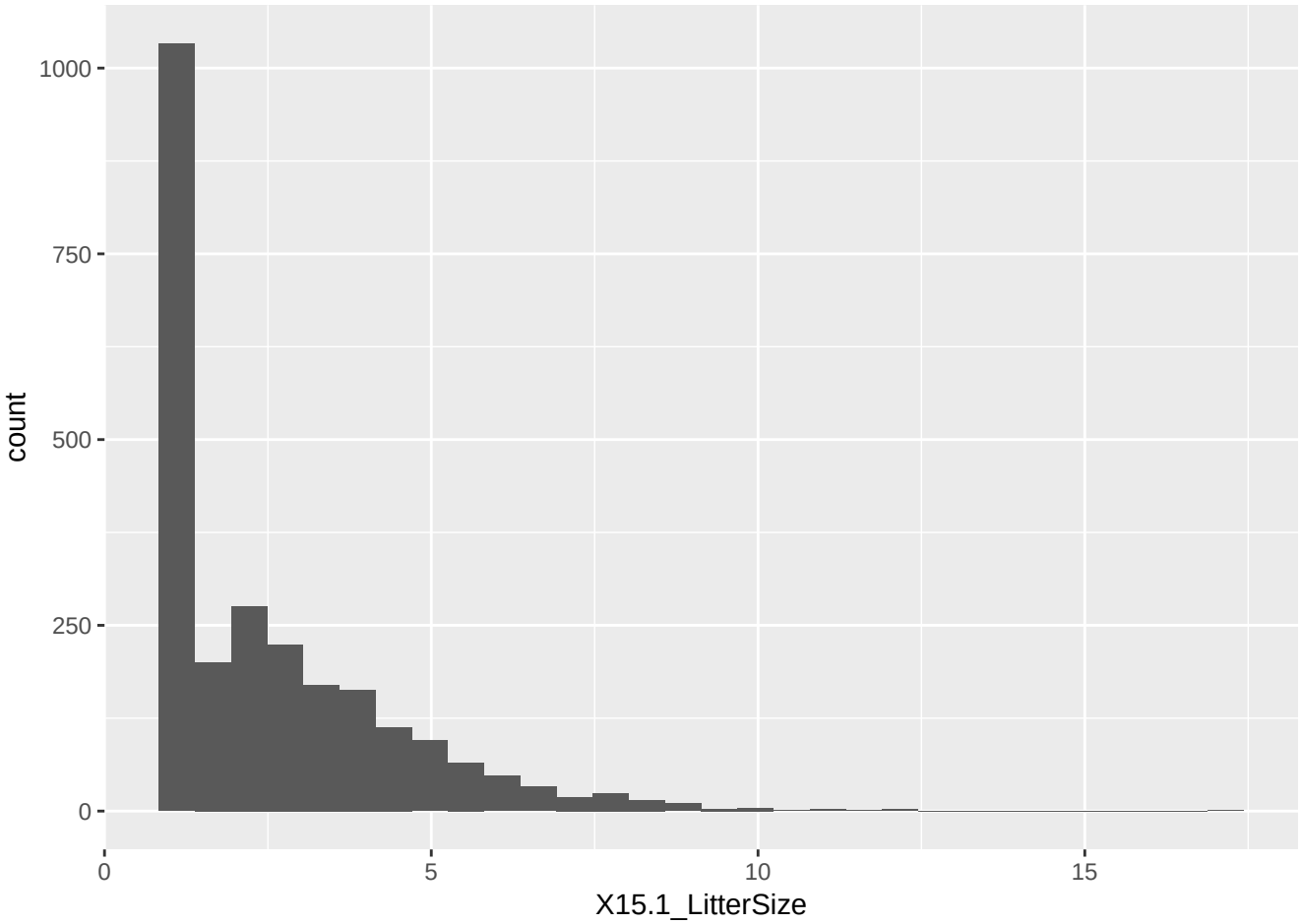
Now we need to choose a variable of interest and make some basic exploratory plots.

```
# Want something with quite a lot of data. Litter size?

sum(!is.na(p$X15.1_LitterSize))
```

```
## [1] 2501
```

```
ggplot(p, aes(X15.1_LitterSize)) + geom_histogram()
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
## Warning: Removed 2915 rows containing non-finite values (stat_bin).
```



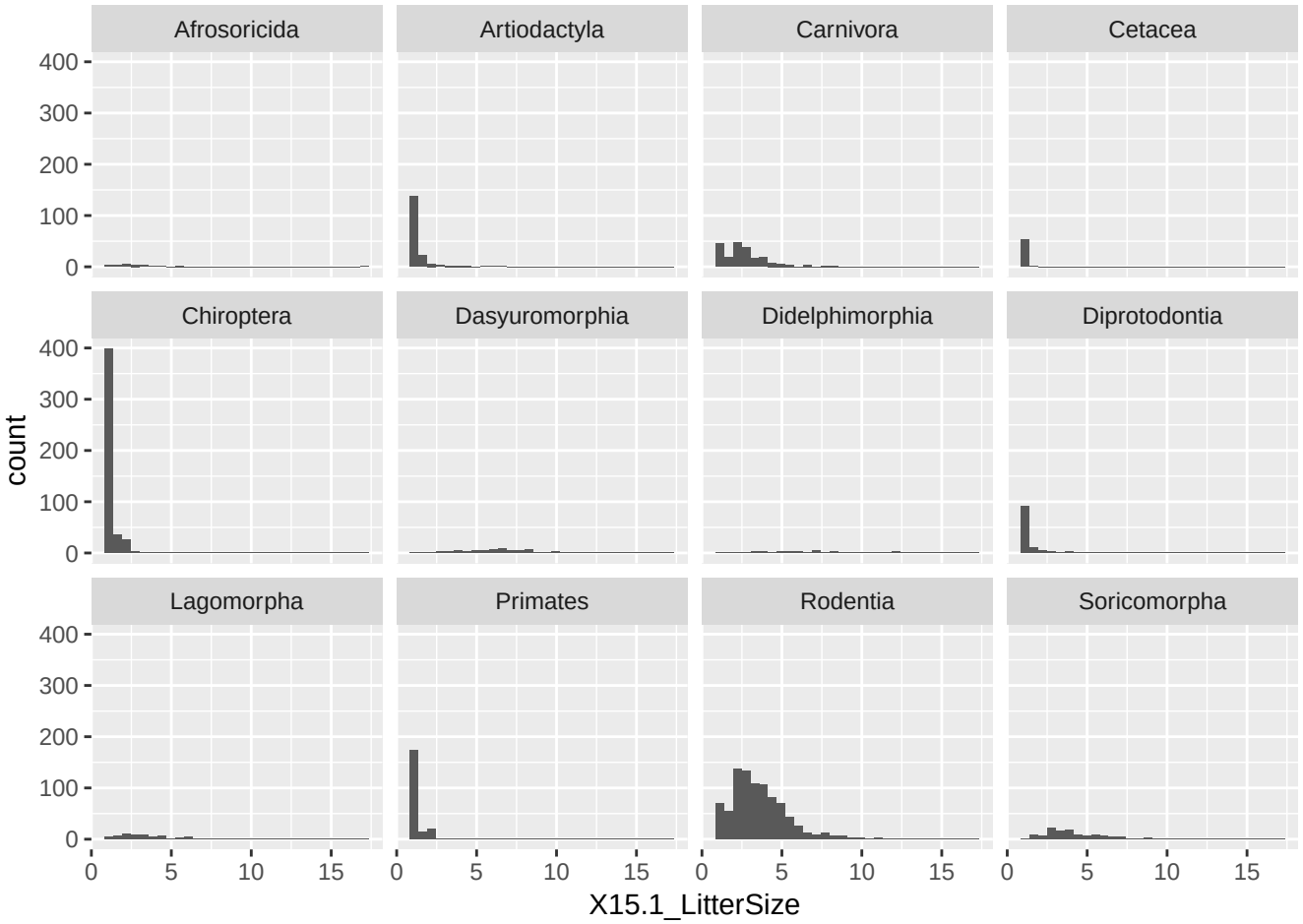

```
p$X15.1_LitterSize %>% summary
```

```
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.    NA's
##   0.840   1.000   1.940   2.523   3.490  16.890    2915
```

```
large_orders <-
  p %>%
    filter(!is.na(sum(!is.na(p$X15.1_LitterSize)))) %>%
    group_by(MSW05_Order) %>%
    count() %>%
    arrange(desc(n)) %>%
    filter(n > 40) %>%
    pull(MSW05_Order)

p %>%
  filter(MSW05_Order %in% large_orders) %>%
  ggplot(aes(X15.1_LitterSize)) +
    geom_histogram() +
    facet_wrap(~ MSW05_Order)
```

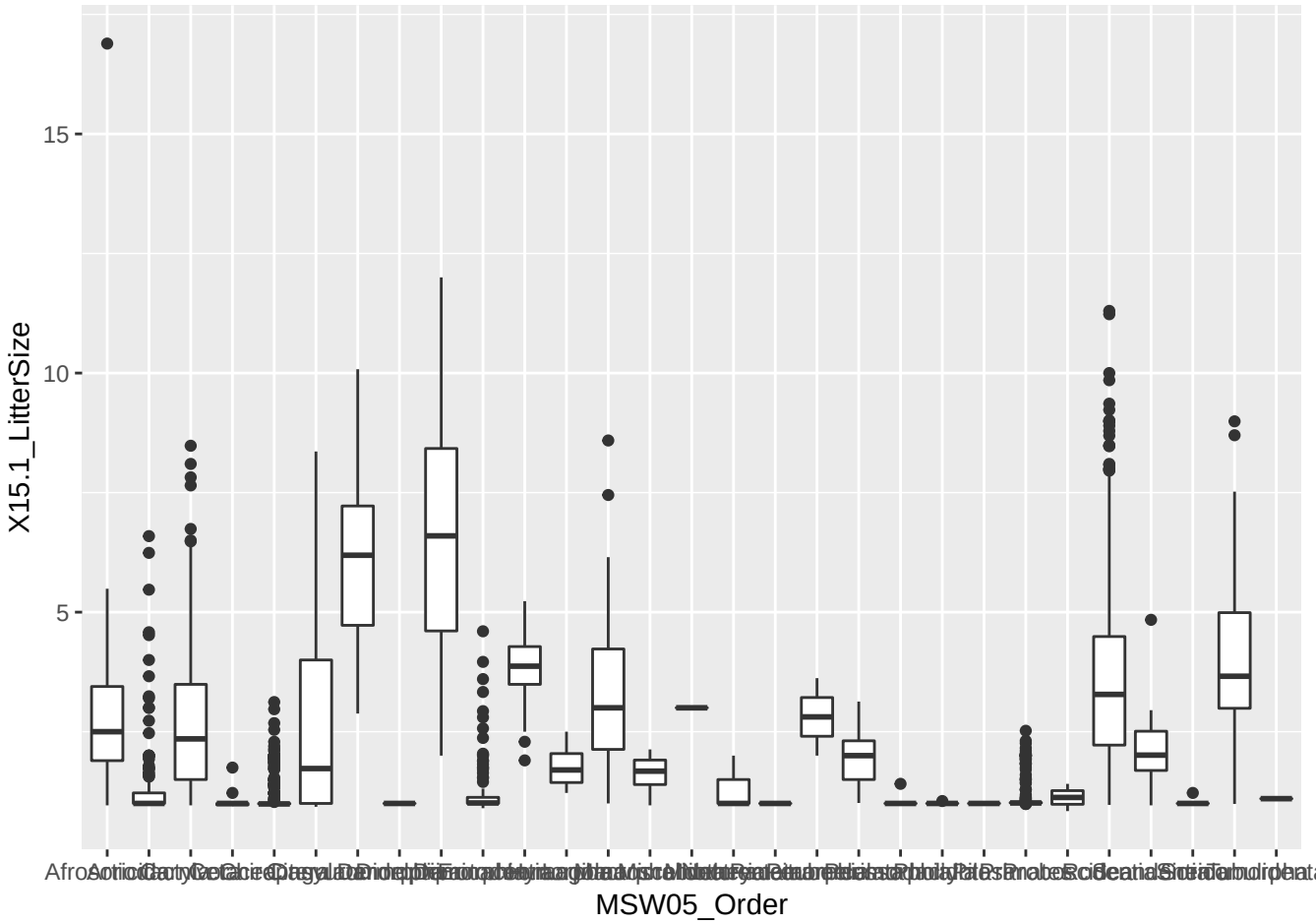
```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

```
## Warning: Removed 2866 rows containing non-finite values (stat_bin).
```



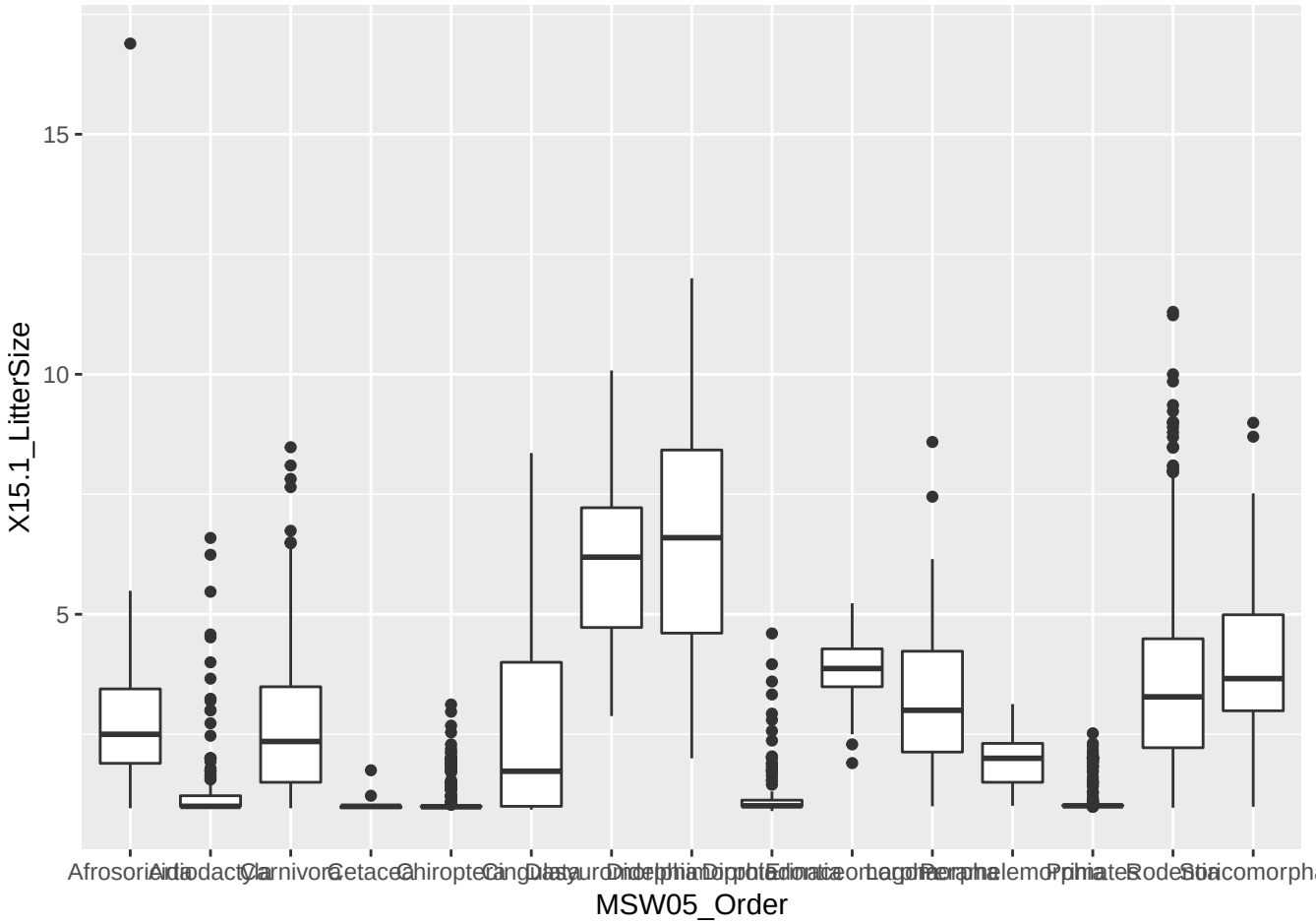

```
ggplot(p, aes(x = MSW05_Order, y = X15.1_LitterSize)) + geom_boxplot()
```

```
## Warning: Removed 2915 rows containing non-finite values (stat_boxplot).
```



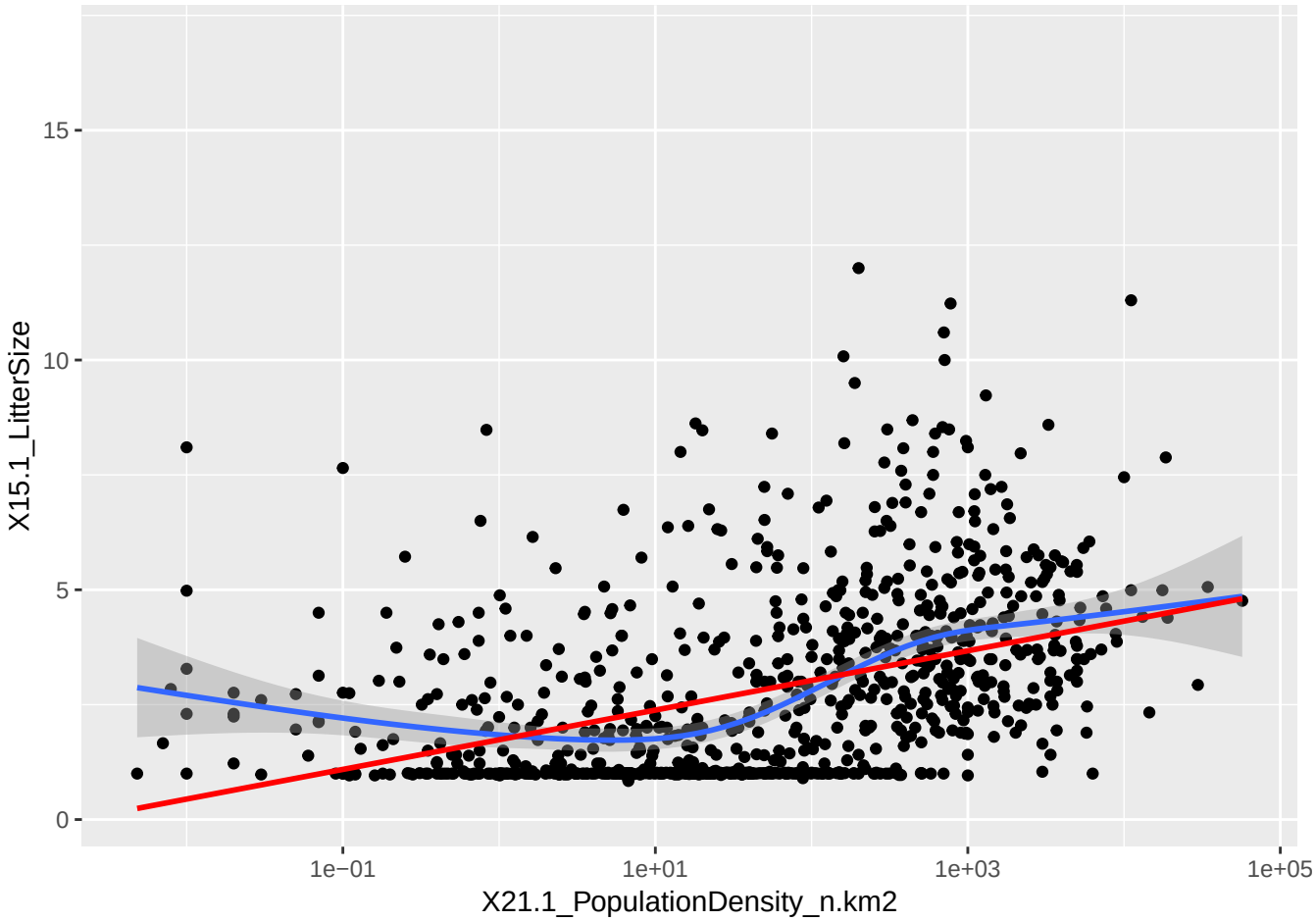

```
p %>%
  group_by(MSW05_Order) %>%
  add_tally %>%
  filter(n > 20) %>%
    ggplot(aes(x = MSW05_Order, y = X15.1_LitterSize)) + geom_boxplot()
```

```
## Warning: Removed 2889 rows containing non-finite values (stat_boxplot).
```




```
## Don't wish to do too many bivariate plots at this point. Going to do a priori variable selection and p valu
ggplot(p, aes(x = X21.1_PopulationDensity_n.km2, y = X15.1_LitterSize)) +
  geom_point() +
  geom_smooth() +
  geom_smooth(method = 'lm', se = FALSE, colour = 'red') +
  scale_x_log10()
```

```
## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
## Warning: Removed 4532 rows containing non-finite values (stat_smooth).
## Warning: Removed 4532 rows containing non-finite values (stat_smooth).
## Warning: Removed 4532 rows containing missing values (geom_point).
```



Some data cleaning

```
# Remove NAs in response and response where litter size is less than one (doesn't make sense).
p <- p %>%
       filter(!is.na(X15.1_LitterSize)) %>%
       filter(X15.1_LitterSize >= 1) %>%
       mutate(y = log1p(X15.1_LitterSize)) %>%
       dplyr::select(-X15.1_LitterSize, -References, -X24.1_TeatNumber)


p_notaxa <- p %>%
              dplyr::select(-contains('MSW05'))

preprocesses <- preProcess(p, method = 'medianImpute')
p_impute <- predict(preprocesses, p_notaxa)
```

Get phylogeny data.

read in phylogeny data.

```
# Read in trees
tree <- read.nexus('https://onlinelibrary.wiley.com/action/downloadSupplement?doi=10.1111%2Fj.1461-0248.2009.0

# Select best supported tree
tree <- tree[[1]]
tree$tip.label <- gsub('_', ' ', tree$tip.label)

# Check if species are available.
mean(p$MSW05_Binomial %in% tree$tip.label)
```

```
## [1] 0.9893813
```

```
in_phylo <- p$MSW05_Binomial %in% tree$tip.label

# Remove data that is not in the phylogeny.

p <- p %>% filter(in_phylo)
p_impute <- p_impute %>% filter(in_phylo)
```

Data summary

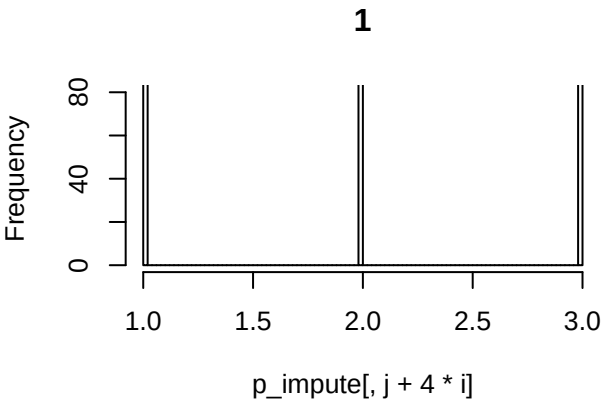
```
dim(p_impute)
```

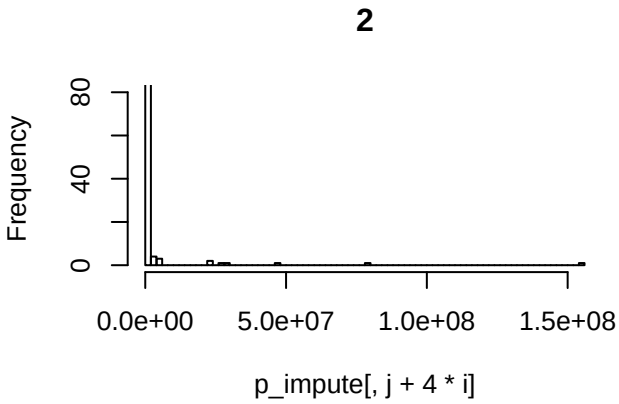
```
## [1] 2143   48
```

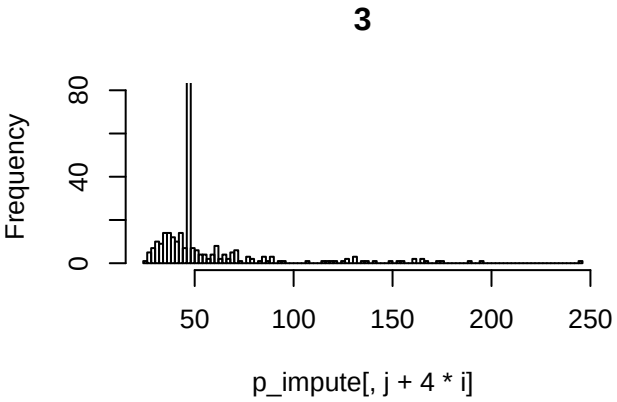
```
names(p_impute)
```

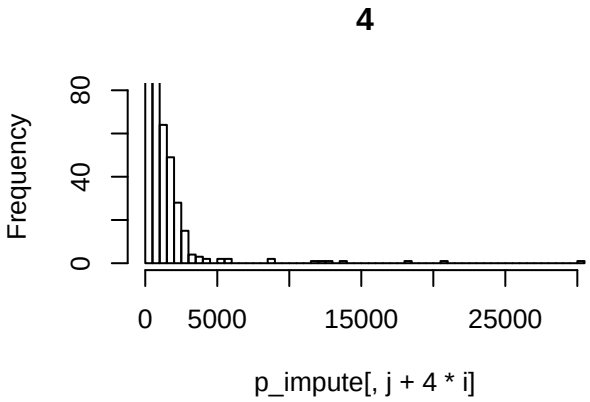
```
##  [1] "X1.1_ActivityCycle"            "X5.1_AdultBodyMass_g"
##  [3] "X8.1_AdultForearmLen_mm"       "X13.1_AdultHeadBodyLen_mm"
##  [5] "X2.1_AgeatEyeOpening_d"        "X3.1_AgeatFirstBirth_d"
##  [7] "X18.1_BasalMetRate_mLO2hr"     "X5.2_BasalMetRateMass_g"
##  [9] "X6.1_DietBreadth"              "X7.1_DispersalAge_d"
## [11] "X9.1_GestationLen_d"           "X12.1_HabitatBreadth"
## [13] "X22.1_HomeRange_km2"           "X22.2_HomeRange_Indiv_km2"
## [15] "X14.1_InterbirthInterval_d"    "X16.1_LittersPerYear"
## [17] "X17.1_MaxLongevity_m"          "X5.3_NeonateBodyMass_g"
## [19] "X13.2_NeonateHeadBodyLen_mm"   "X21.1_PopulationDensity_n.km2"
## [21] "X10.1_PopulationGrpSize"       "X23.1_SexualMaturityAge_d"
## [23] "X10.2_SocialGrpSize"           "X12.2_Terrestriality"
## [25] "X6.2_TrophicLevel"             "X25.1_WeaningAge_d"
## [27] "X5.4_WeaningBodyMass_g"        "X13.3_WeaningHeadBodyLen_mm"
## [29] "X5.5_AdultBodyMass_g_EXT"      "X16.2_LittersPerYear_EXT"
## [31] "X5.6_NeonateBodyMass_g_EXT"    "X5.7_WeaningBodyMass_g_EXT"
## [33] "X26.1_GR_Area_km2"             "X26.2_GR_MaxLat_dd"
## [35] "X26.3_GR_MinLat_dd"            "X26.4_GR_MidRangeLat_dd"
## [37] "X26.5_GR_MaxLong_dd"           "X26.6_GR_MinLong_dd"
## [39] "X26.7_GR_MidRangeLong_dd"      "X27.1_HuPopDen_Min_n.km2"
## [41] "X27.2_HuPopDen_Mean_n.km2"     "X27.3_HuPopDen_5p_n.km2"
## [43] "X27.4_HuPopDen_Change"         "X28.1_Precip_Mean_mm"
## [45] "X28.2_Temp_Mean_01degC"        "X30.1_AET_Mean_mm"
## [47] "X30.2_PET_Mean_mm"             "y"
```

```
par(mfrow = c(2, 2))

for(i in 0:11){
  for( j in 1:4){

    if(j + 4 * i <= ncol(p_impute)){
      hist(p_impute[, j + 4 * i], breaks = 100, ylim = c(0, 80), main = j + 4 * i)
    }

  }
  print(i)
  par(mfrow = c(2, 2))
}
```

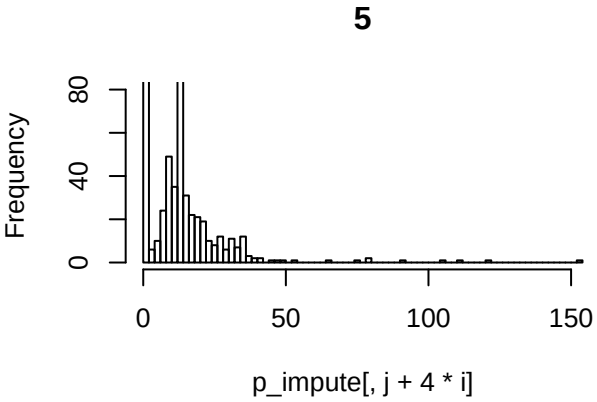

1
Frequency
0
40
80
1.0
1.5
2.0
2.5
3.0
p_impute[, j + 4 * i]

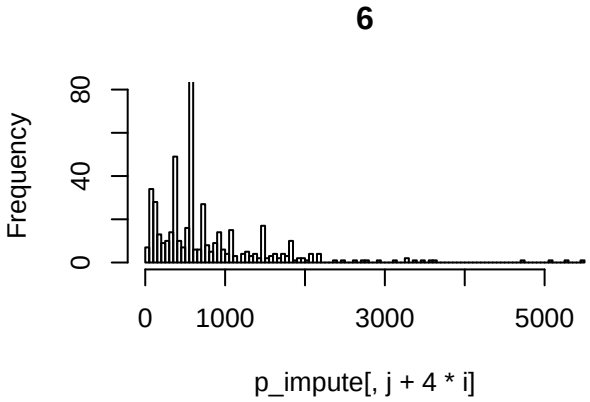

2
Frequency
0
40
80
0.0e+00
5.0e+07
1.0e+08
1.5e+08
p_impute[, j + 4 * i]

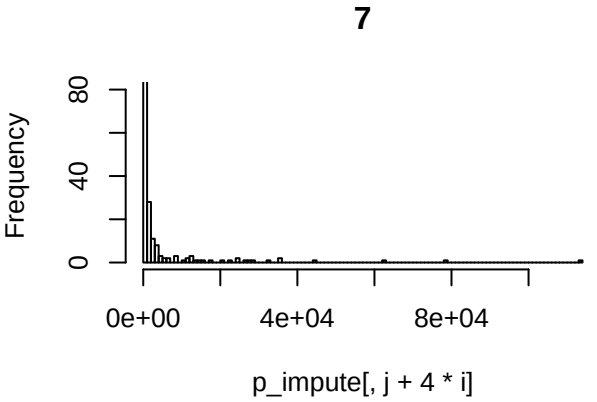

3
Frequency
0
40
80
50
100
150
200
250
p_impute[, j + 4 * i]

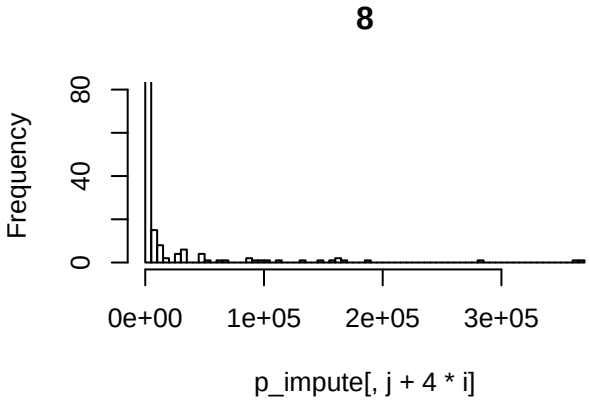

4
Frequency
0
40
80
0
5000
15000
25000
p_impute[, j + 4 * i]

```
## [1] 0
```

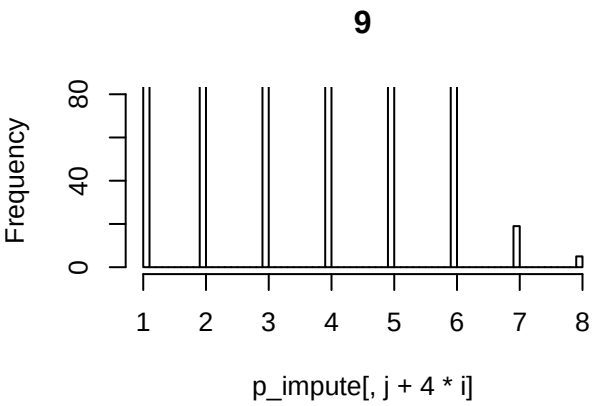

5
Frequency
0
40
80
0
50
100
150
p_impute[, j + 4 * i]

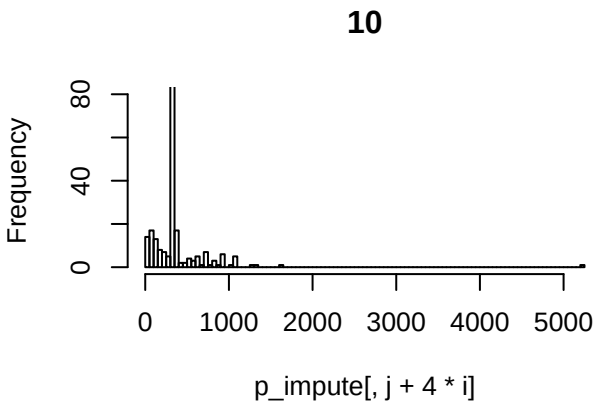

6
Frequency
0
40
80
0
1000
3000
5000
p_impute[, j + 4 * i]

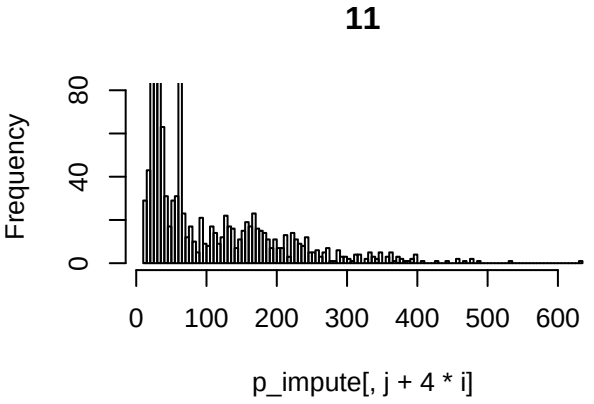

7
Frequency
0
40
80
0e+00
4e+04
8e+04
p_impute[, j + 4 * i]

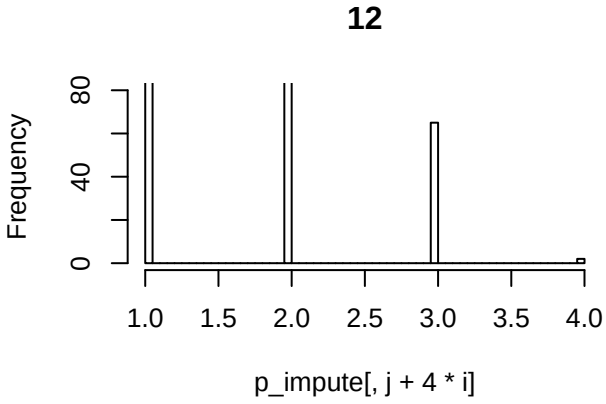

8
Frequency
0
40
80
0e+00
1e+05
2e+05
3e+05
p_impute[, j + 4 * i]

```
## [1] 1
```

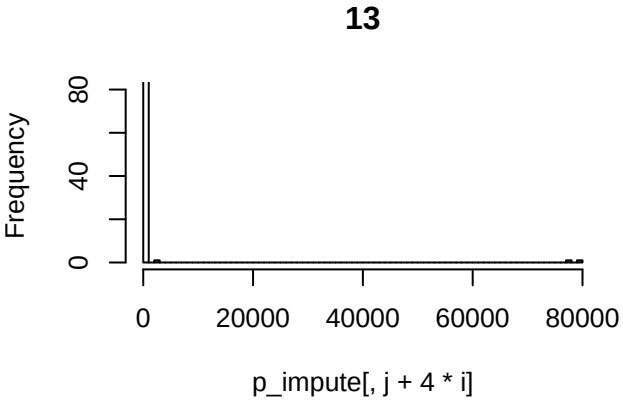

9
Frequency
0
40
80
1
2
3
4
5
6
7
8
p_impute[, j + 4 * i]

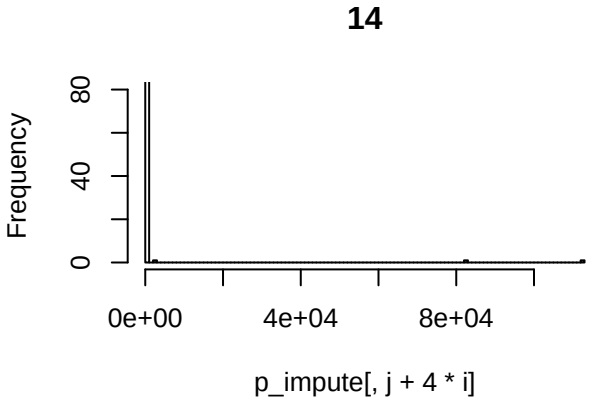

10
Frequency
0
40
80
0
1000
2000
3000
4000
5000
p_impute[, j + 4 * i]

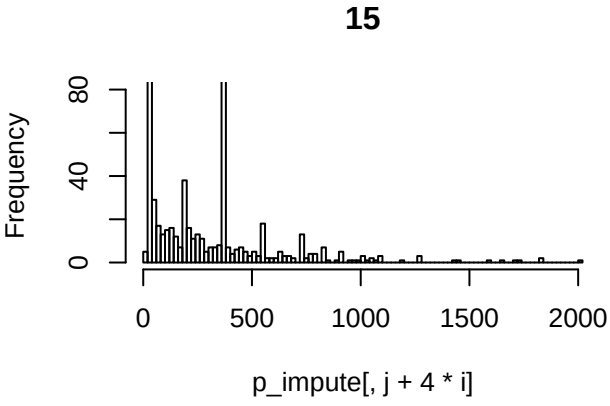

11
Frequency
0
40
80
0
100
200
300
400
500
600
p_impute[, j + 4 * i]

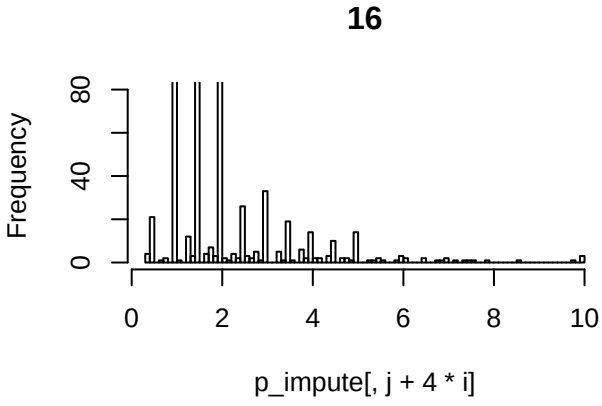

12
Frequency
0
40
80
1.0
1.5
2.0
2.5
3.0
3.5
4.0
p_impute[, j + 4 * i]

```
## [1] 2
```

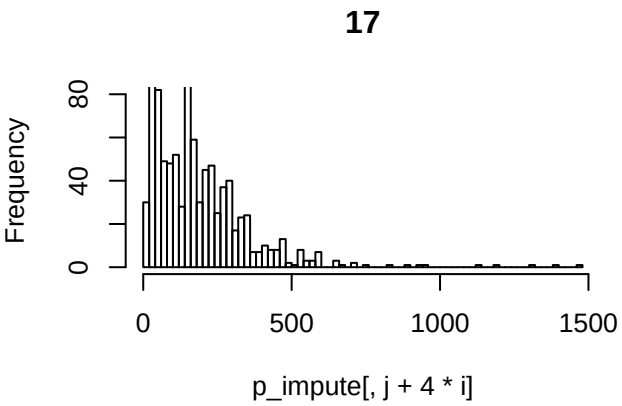

13
Frequency
0
40
80
0
20000
40000
60000
80000
p_impute[, j + 4 * i]

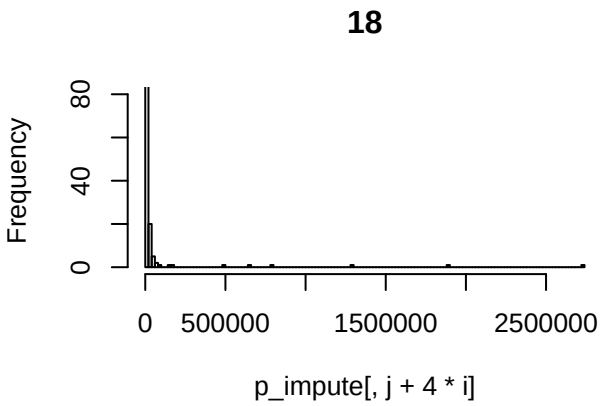

14
Frequency
0
40
80
0e+00
4e+04
8e+04
p_impute[, j + 4 * i]

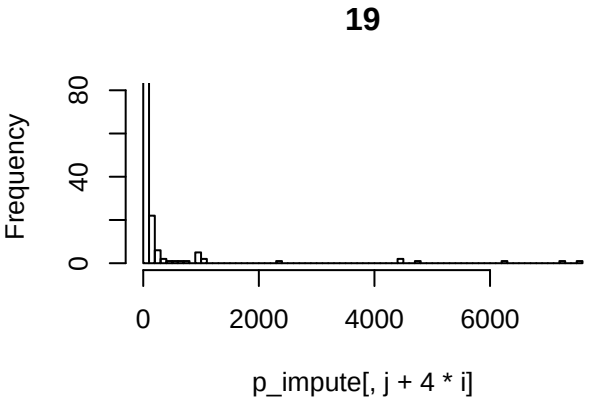

15
Frequency
0
40
80
0
500
1000
1500
2000
p_impute[, j + 4 * i]

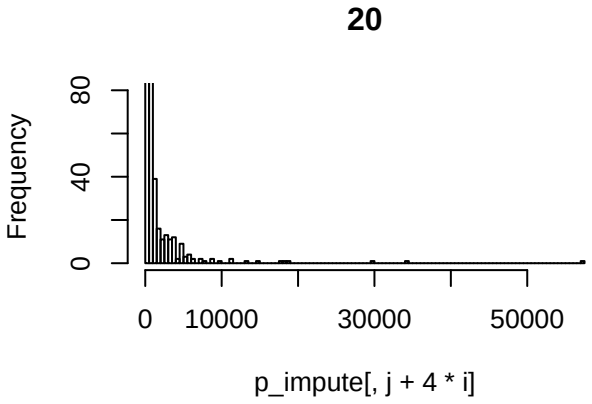

16
Frequency
0
40
80
0
2
4
6
8
10
p_impute[, j + 4 * i]

```
## [1] 3
```

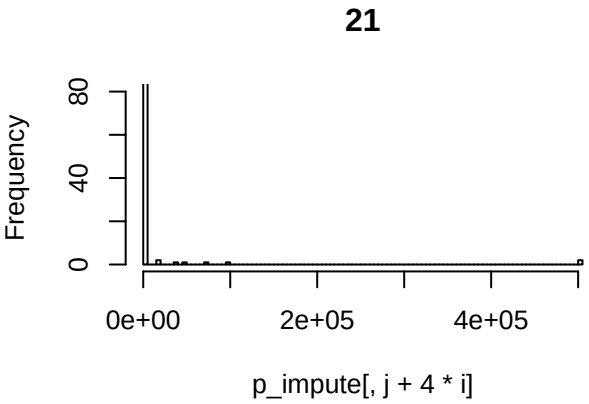

17
Frequency
0
40
80
0
500
1000
1500
p_impute[, j + 4 * i]

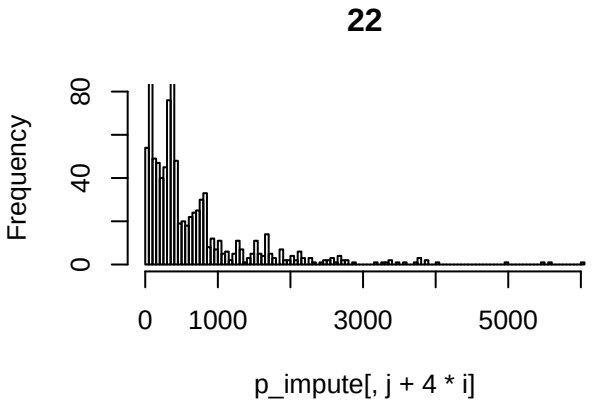

18
Frequency
0
40
80
0
500000
1500000
2500000
p_impute[, j + 4 * i]

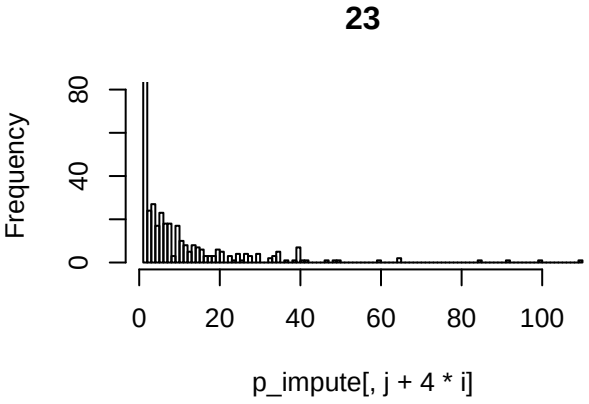

19
Frequency
0
40
80
0
2000
4000
6000
p_impute[, j + 4 * i]

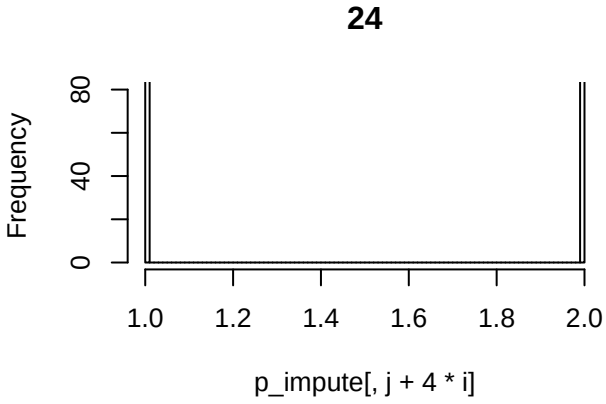

20
Frequency
0
40
80
0
10000
30000
50000
p_impute[, j + 4 * i]

```
## [1] 4
```

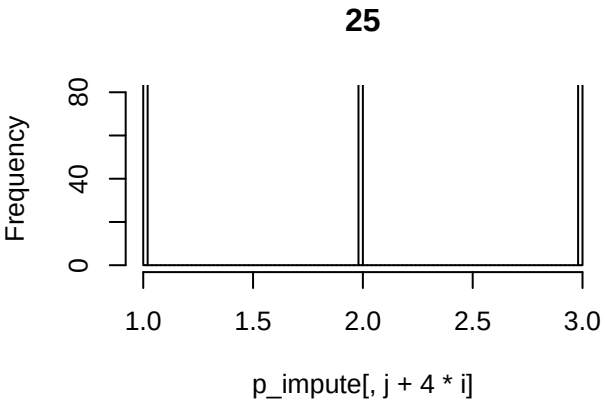

21
Frequency
0
40
80
0e+00
2e+05
4e+05
p_impute[, j + 4 * i]

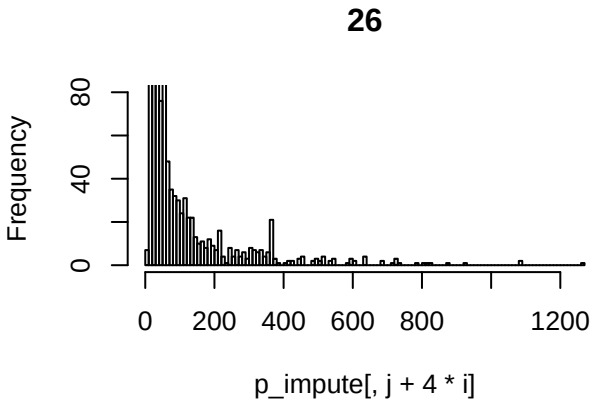

22
Frequency
0
40
80
0
1000
3000
5000
p_impute[, j + 4 * i]

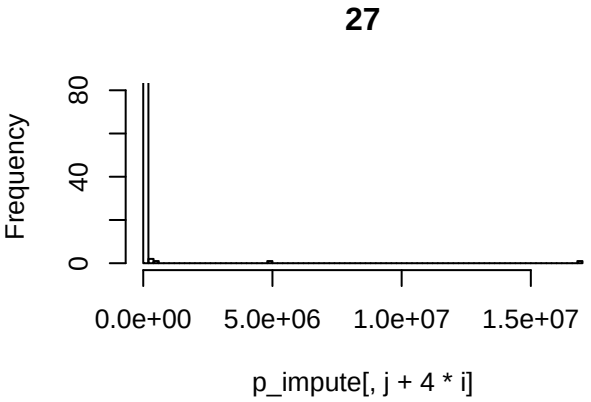

23
Frequency
0
40
80
0
20
40
60
80
100
p_impute[, j + 4 * i]

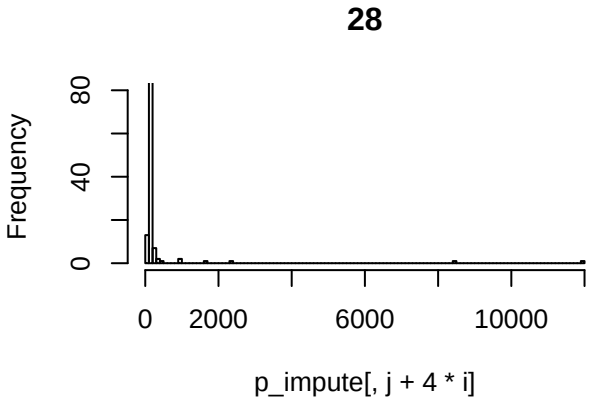

24
Frequency
0
40
80
1.0
1.2
1.4
1.6
1.8
2.0
p_impute[, j + 4 * i]

```
## [1] 5
```

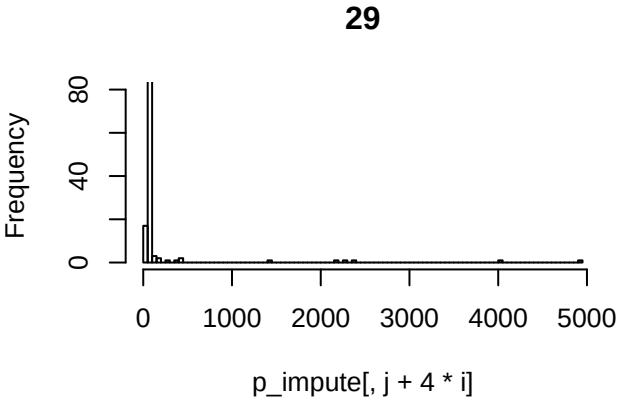

25
Frequency
0
40
80
1.0
1.5
2.0
2.5
3.0
p_impute[, j + 4 * i]

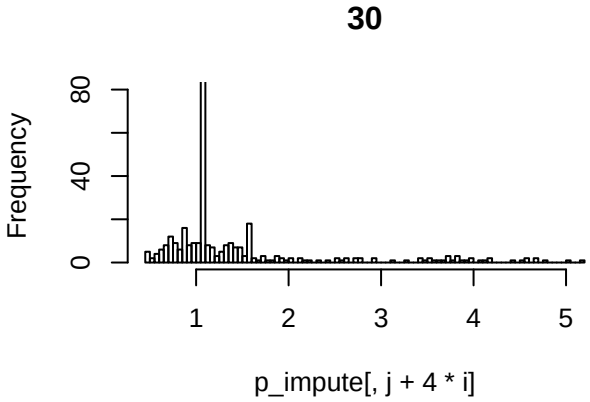

26
Frequency
0
40
80
0
200
400
600
800
1200
p_impute[, j + 4 * i]

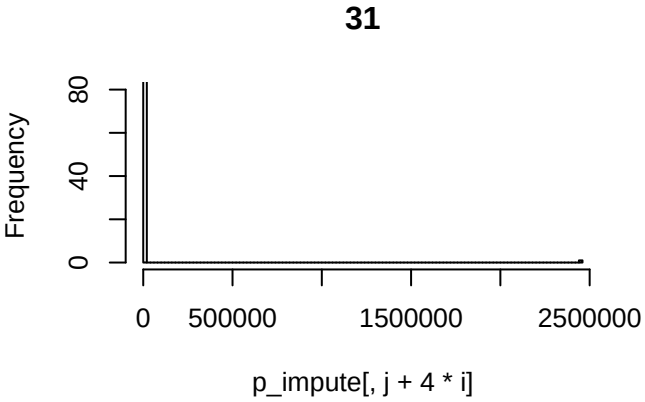

27
Frequency
0
40
80
0.0e+00
5.0e+06
1.0e+07
1.5e+07
p_impute[, j + 4 * i]

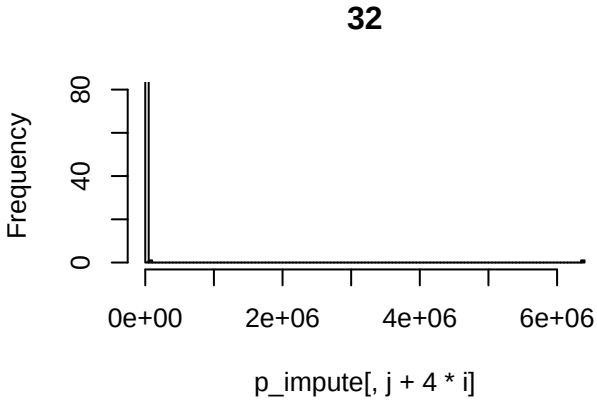

28
Frequency
0
40
80
0
2000
6000
10000
p_impute[, j + 4 * i]

```
## [1] 6
```

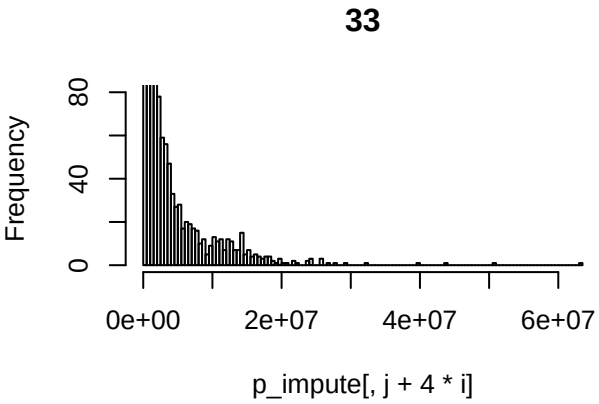

29
Frequency
0
40
80
0
1000
2000
3000
4000
5000
p_impute[, j + 4 * i]

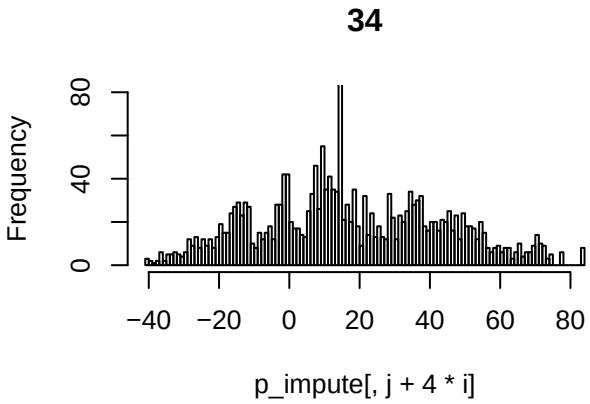

30
Frequency
0
40
80
1
2
3
4
5
p_impute[, j + 4 * i]

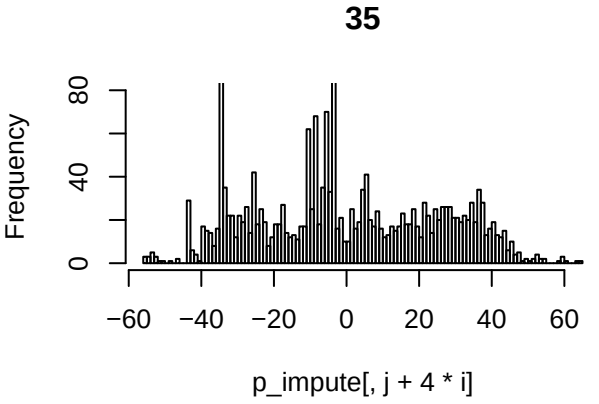

31
Frequency
0
40
80
0
500000
1500000
2500000
p_impute[, j + 4 * i]

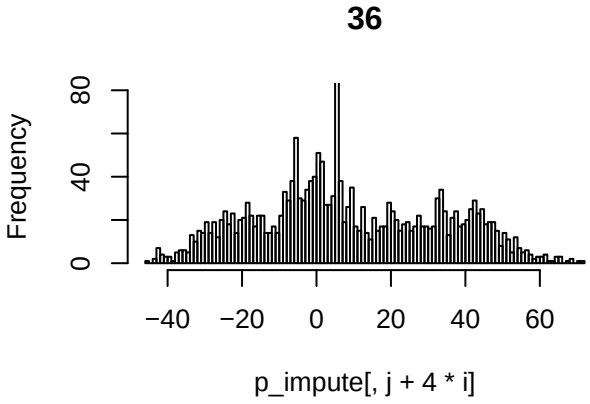

32
Frequency
0
40
80
0e+00
2e+06
4e+06
6e+06
p_impute[, j + 4 * i]

```
## [1] 7
```

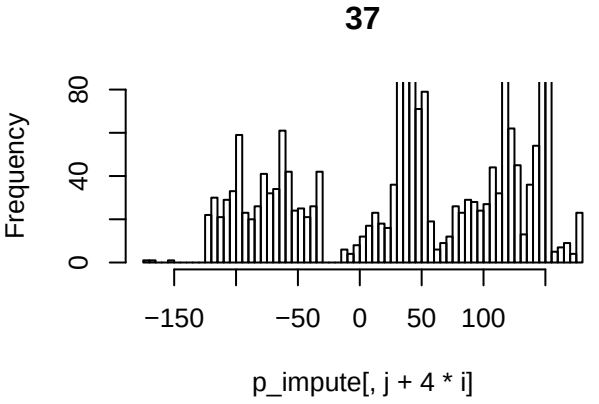

33
Frequency
0
40
80
0e+00
2e+07
4e+07
6e+07
p_impute[, j + 4 * i]

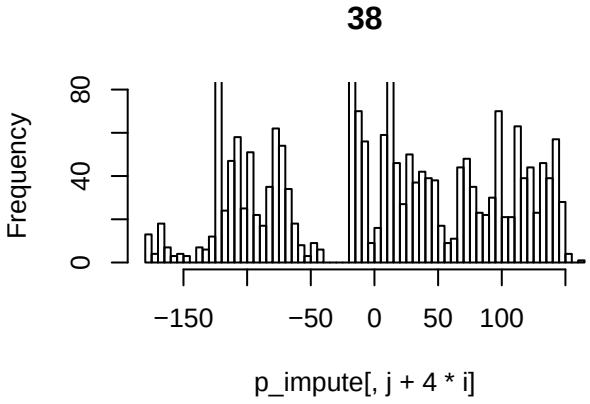

34
Frequency
0
40
80
−40
−20
0
20
40
60
80
p_impute[, j + 4 * i]

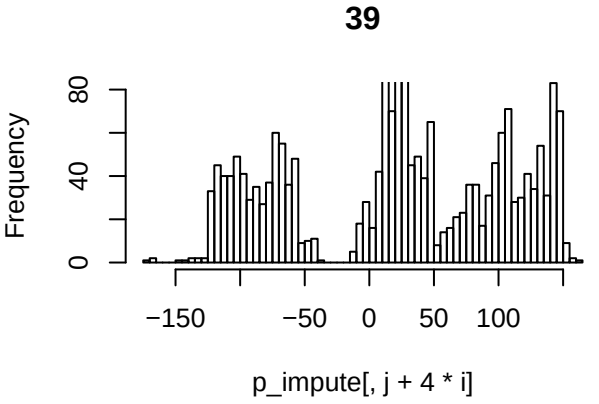

35
Frequency
0
40
80
−60
−40
−20
0
20
40
60
p_impute[, j + 4 * i]

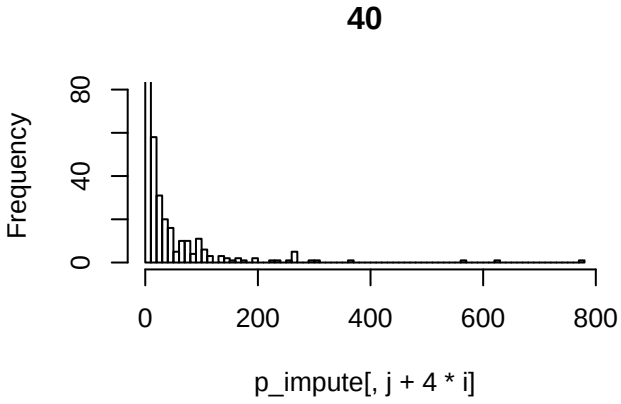

36
Frequency
0
40
80
−40
−20
0
20
40
60
p_impute[, j + 4 * i]

```
## [1] 8
```

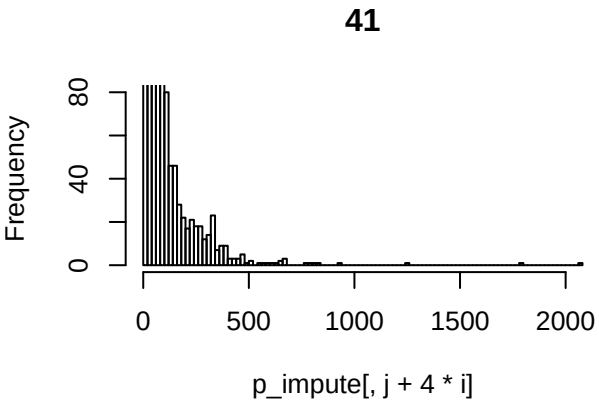

37
Frequency
0
40
80
−150
−50
0
50
100
p_impute[, j + 4 * i]

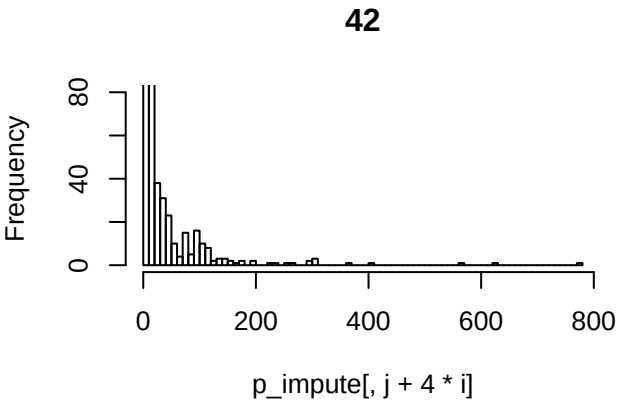

38
Frequency
0
40
80
−150
−50
0
50
100
p_impute[, j + 4 * i]

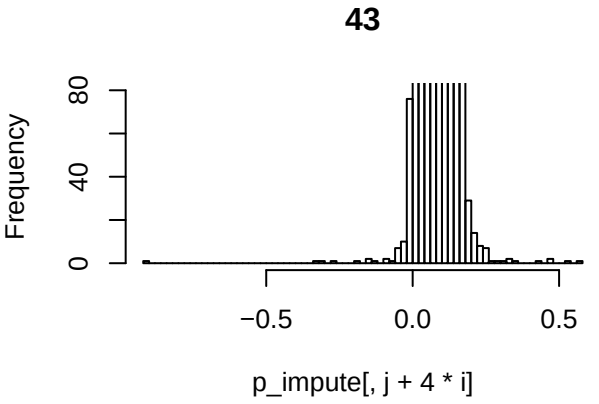

39
Frequency
0
40
80
−150
−50
0
50
100
p_impute[, j + 4 * i]

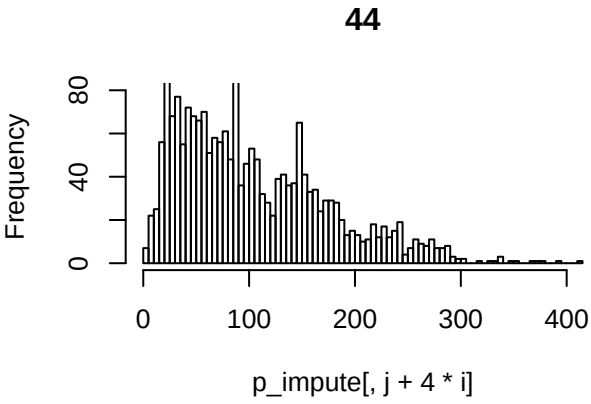

40
Frequency
0
40
80
0
200
400
600
800
p_impute[, j + 4 * i]

```
## [1] 9
```

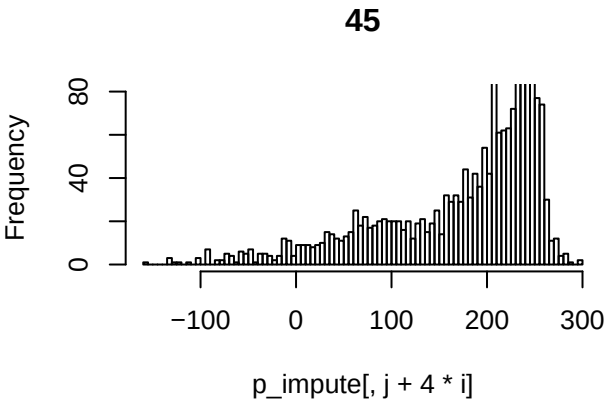

41
Frequency
0
40
80
0
500
1000
1500
2000
p_impute[, j + 4 * i]

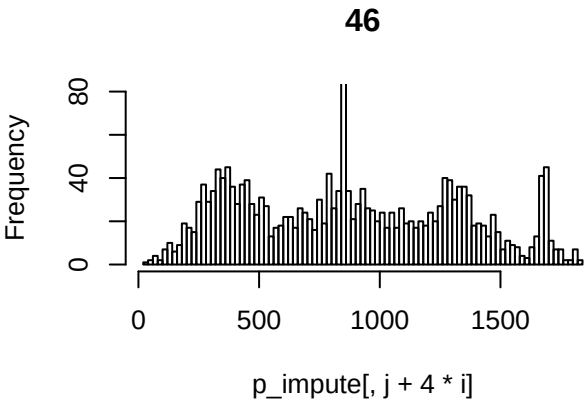

42
Frequency
0
40
80
0
200
400
600
800
p_impute[, j + 4 * i]

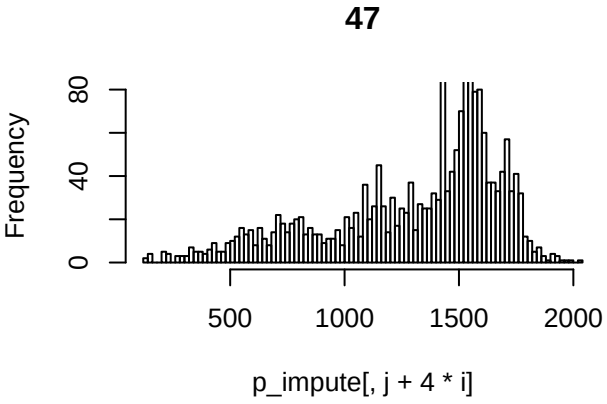

43
Frequency
0
40
80
−0.5
0.0
0.5
p_impute[, j + 4 * i]

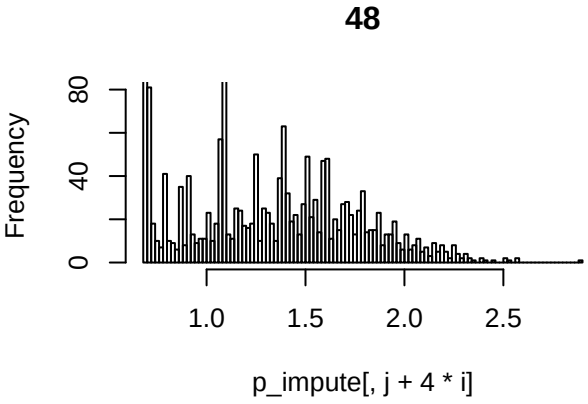

44
Frequency
0
40
80
0
100
200
300
400
p_impute[, j + 4 * i]

```
## [1] 10
```


45
Frequency
0
40
80
−100
0
100
200
300
p_impute[, j + 4 * i]


46
Frequency
0
40
80
0
500
1000
1500
p_impute[, j + 4 * i]

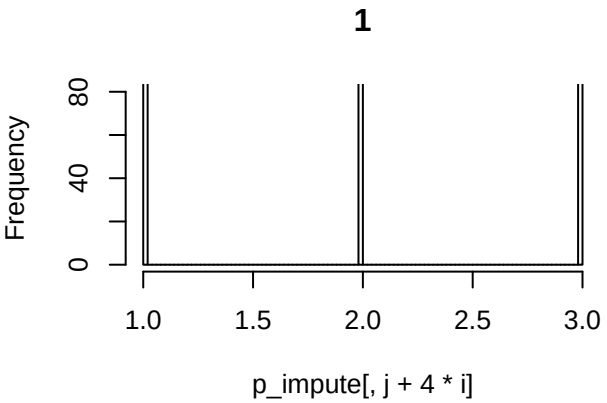

47
Frequency
0
40
80
500
1000
1500
2000
p_impute[, j + 4 * i]

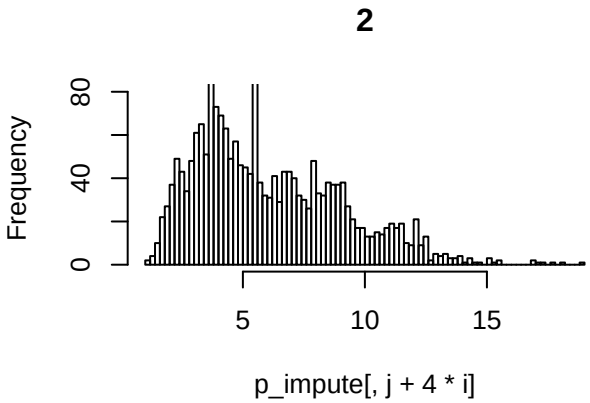

48
Frequency
0
40
80
1.0
1.5
2.0
2.5
p_impute[, j + 4 * i]

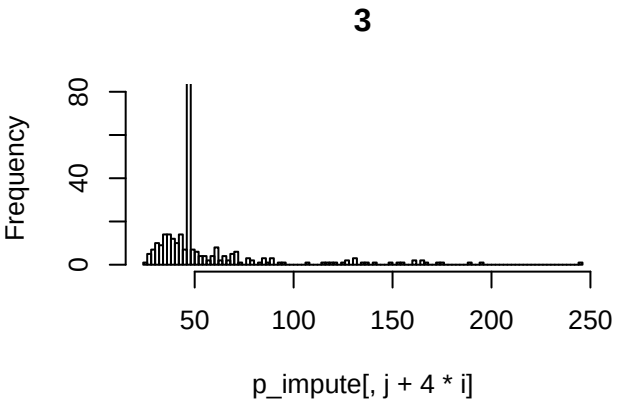
```
## [1] 11
```

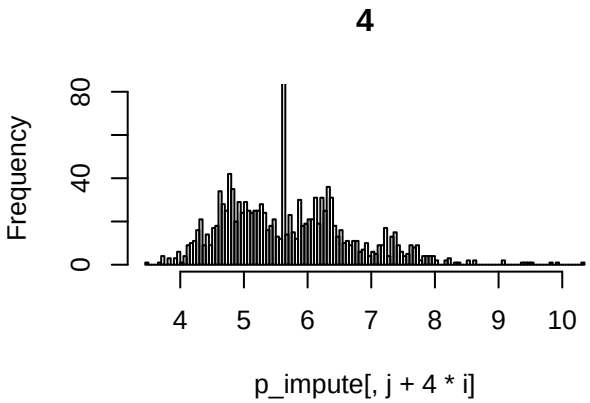
Log Transforms

```
log_cols <- c(2, 4, 7, 8,
              10, 11, 13, 14, 15, 17, 18, 19,
              20, 21, 22, 23, 26, 27, 28, 29,
              31, 32, 33,
              40, 41, 42)

p_impute[, log_cols] <- log1p(p_impute[, log_cols])


par(mfrow = c(2, 2))

for(i in 0:11){
  for( j in 1:4){

    if(j + 4 * i <= ncol(p_impute)){
      hist(p_impute[, j + 4 * i], breaks = 100, ylim = c(0, 80), main = j + 4 * i)
    }

  }
  print(i)
  par(mfrow = c(2, 2))
}
```

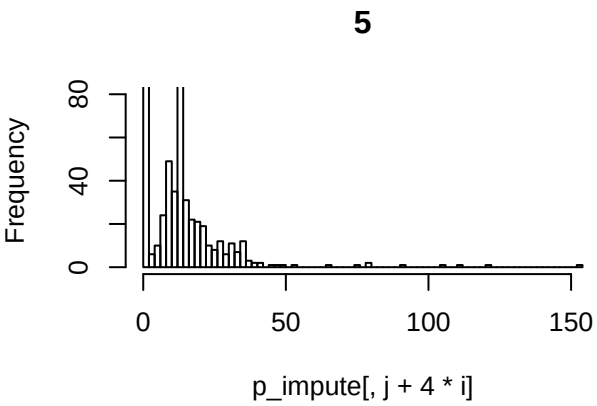


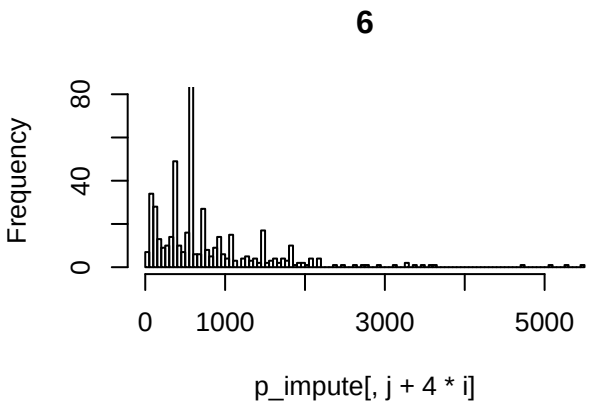


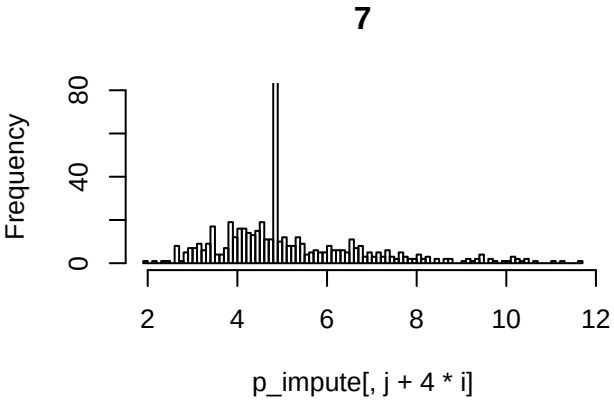


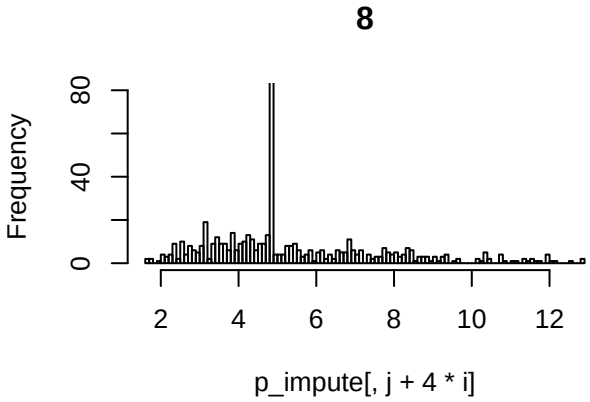



```
## [1] 0
```

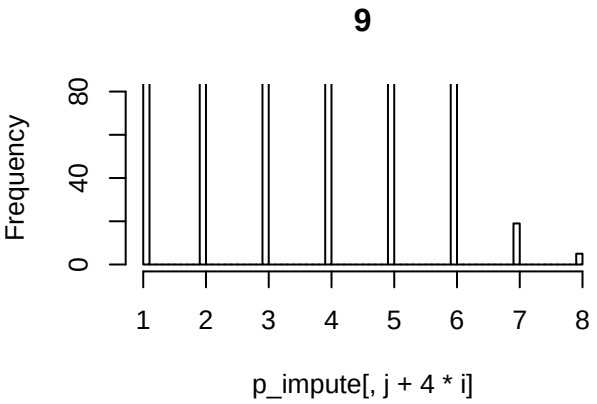

5
Frequency
0
40
80
0
50
100
150
p_impute[, j + 4 * i]

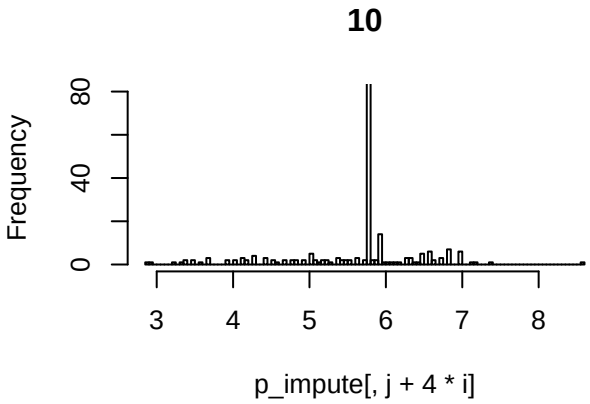

6
Frequency
0
40
80
0
1000
3000
5000
p_impute[, j + 4 * i]

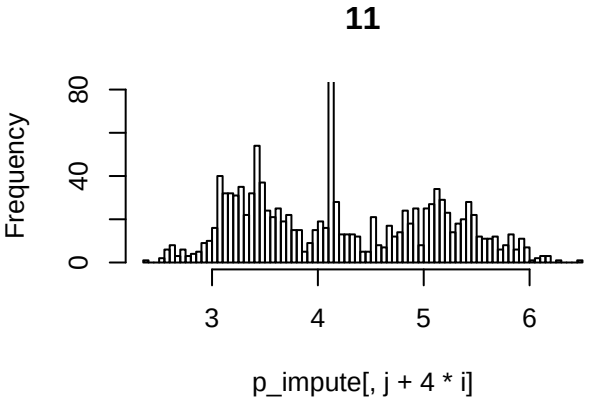

7
Frequency
0
40
80
2
4
6
8
10
12
p_impute[, j + 4 * i]

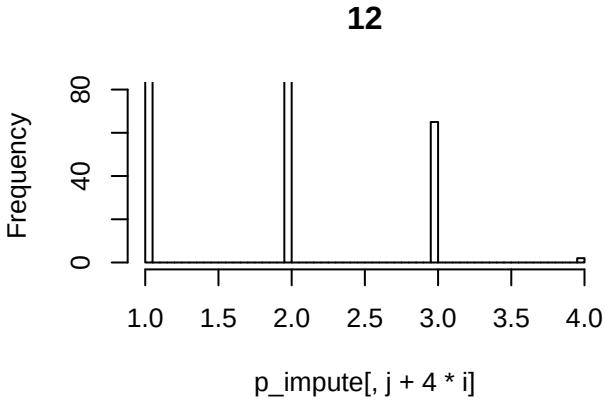

8
Frequency
0
40
80
2
4
6
8
10
12
p_impute[, j + 4 * i]

```
## [1] 1
```

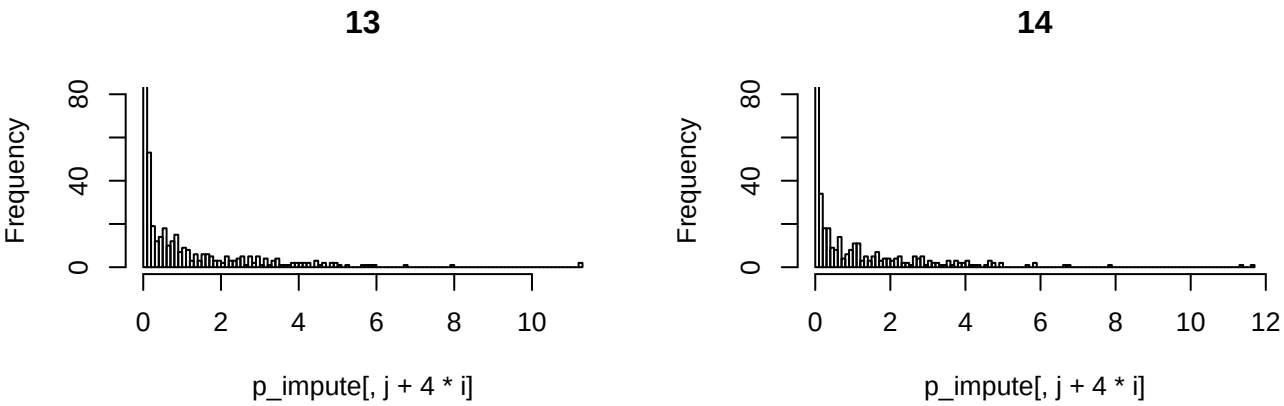

9
Frequency
0
40
80
1
2
3
4
5
6
7
8
p_impute[, j + 4 * i]


10
Frequency
0
40
80
3
4
5
6
7
8
p_impute[, j + 4 * i]

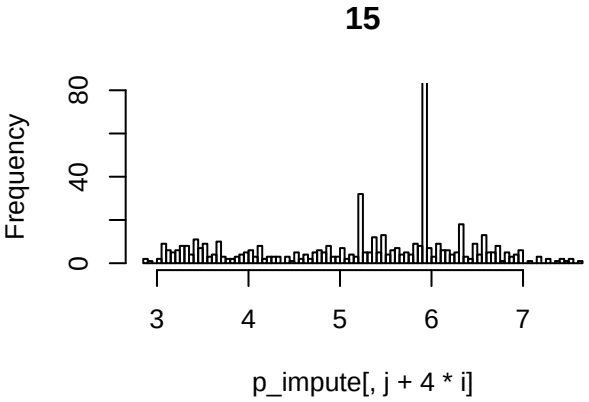

11
Frequency
0
40
80
3
4
5
6
p_impute[, j + 4 * i]

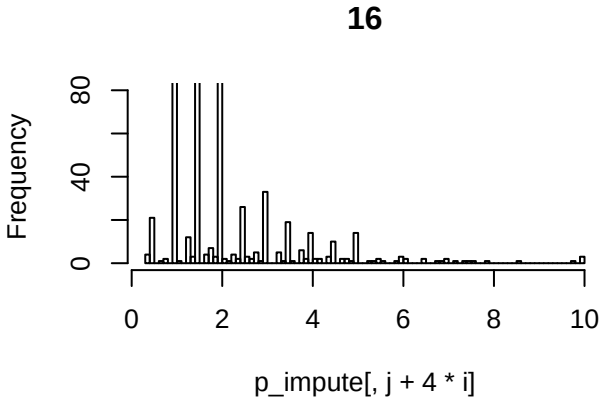

12
Frequency
0
40
80
1.0
1.5
2.0
2.5
3.0
3.5
4.0
p_impute[, j + 4 * i]

```
## [1] 2
```

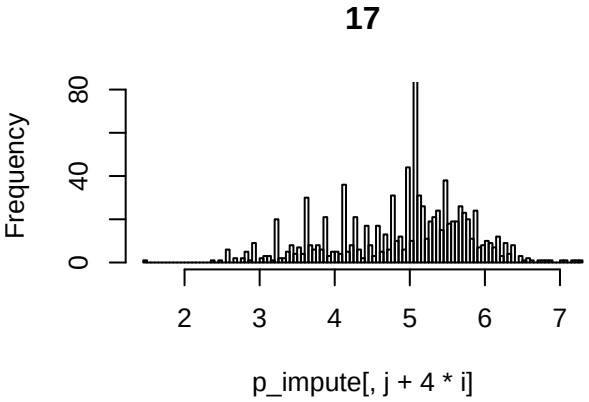

13
Frequency
0
40
80
0
2
4
6
8
10
p_impute[, j + 4 * i]

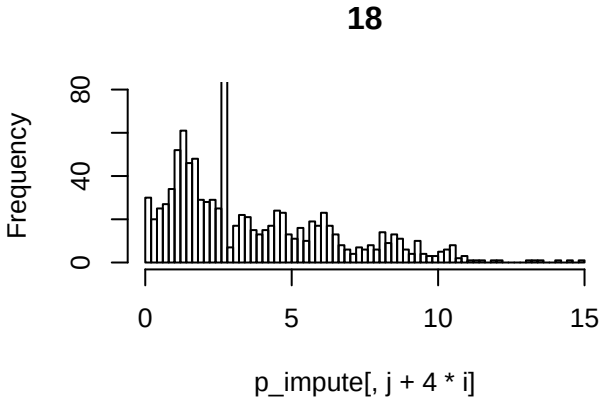
14
Frequency
0
40
80
0
2
4
6
8
10
12
p_impute[, j + 4 * i]

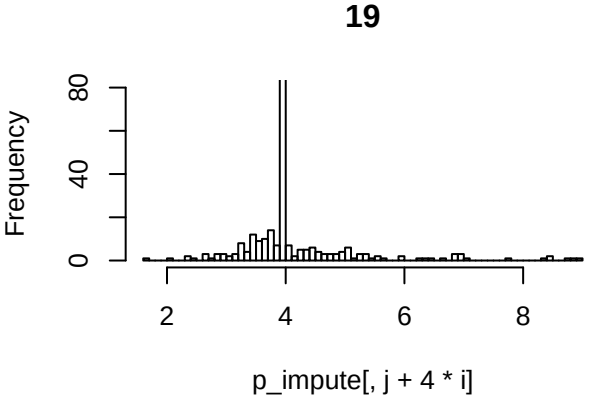

15
Frequency
0
40
80
3
4
5
6
7
p_impute[, j + 4 * i]

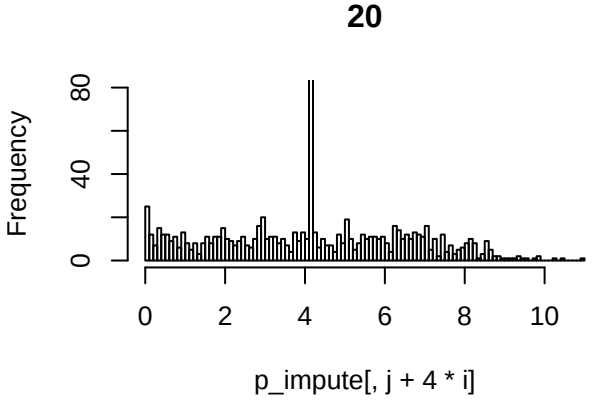

16
Frequency
0
40
80
0
2
4
6
8
10
p_impute[, j + 4 * i]

```
## [1] 3
```

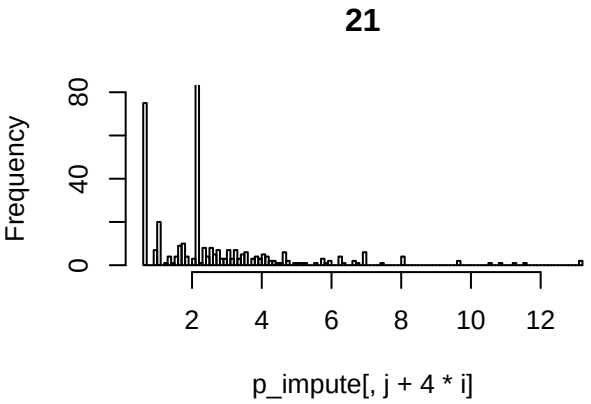

17
Frequency
0
40
80
2
3
4
5
6
7
p_impute[, j + 4 * i]

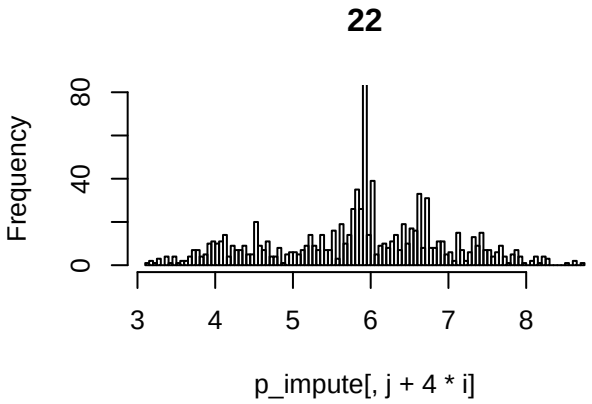

18
Frequency
0
40
80
0
5
10
15
p_impute[, j + 4 * i]

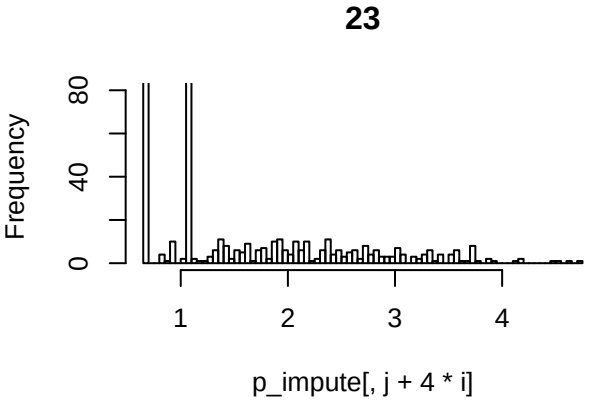

19
Frequency
0
40
80
2
4
6
8
p_impute[, j + 4 * i]

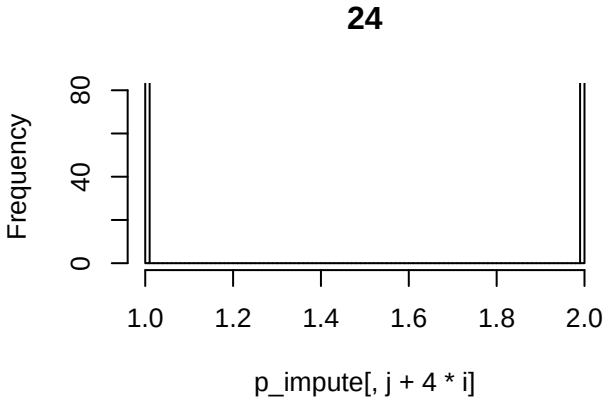

20
Frequency
0
40
80
0
2
4
6
8
10
p_impute[, j + 4 * i]

```
## [1] 4
```

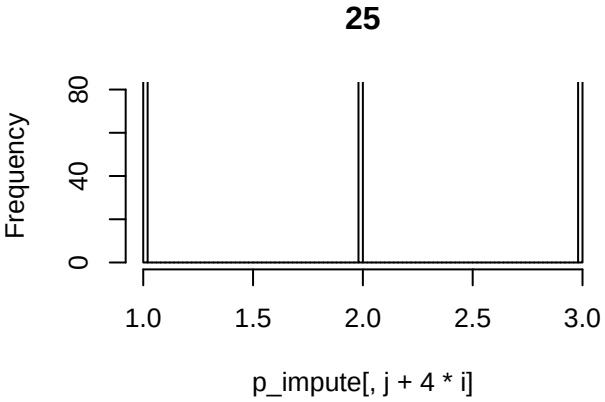

21
Frequency
0
40
80
2
4
6
8
10
12
p_impute[, j + 4 * i]

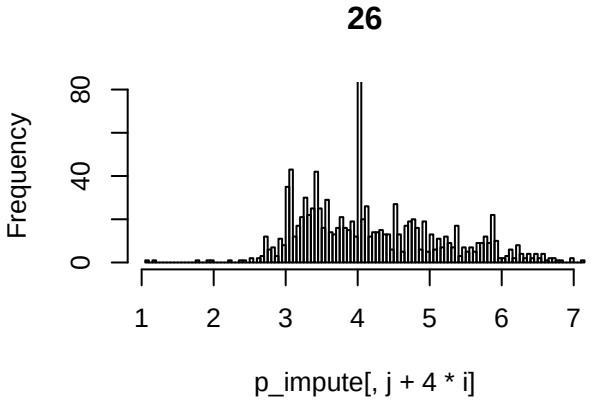

22
Frequency
0
40
80
3
4
5
6
7
8
p_impute[, j + 4 * i]

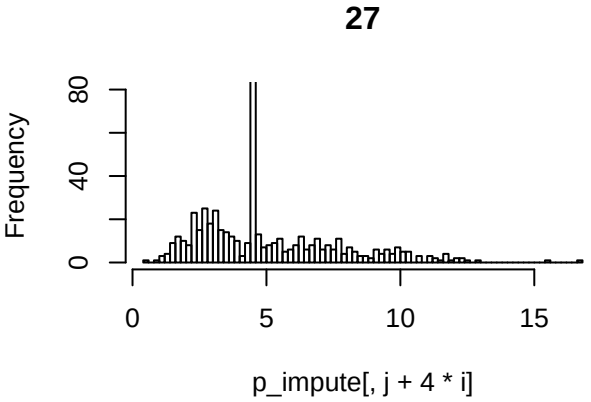

23
Frequency
0
40
80
1
2
3
4
p_impute[, j + 4 * i]

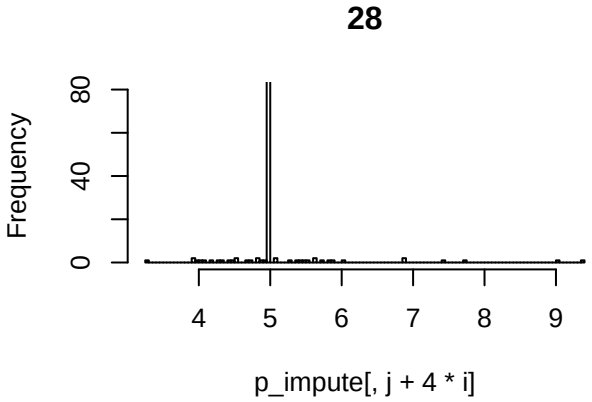

24
Frequency
0
40
80
1.0
1.2
1.4
1.6
1.8
2.0
p_impute[, j + 4 * i]

```
## [1] 5
```

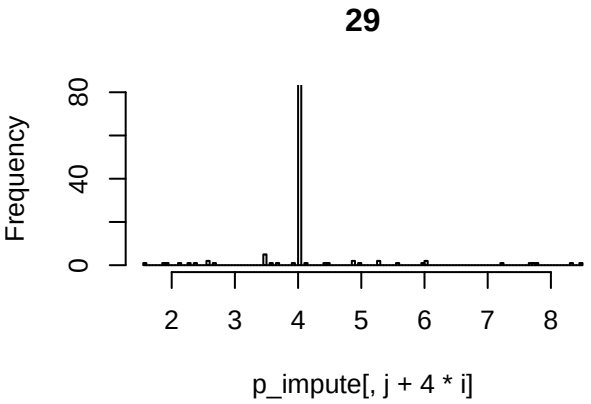

25
Frequency
0
40
80
1.0
1.5
2.0
2.5
3.0
p_impute[, j + 4 * i]

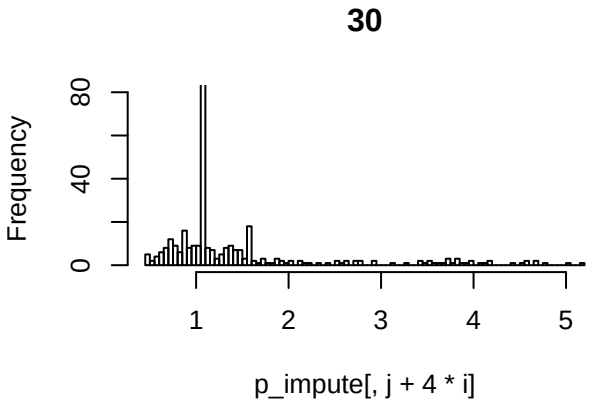

26
Frequency
0
40
80
1
2
3
4
5
6
7
p_impute[, j + 4 * i]

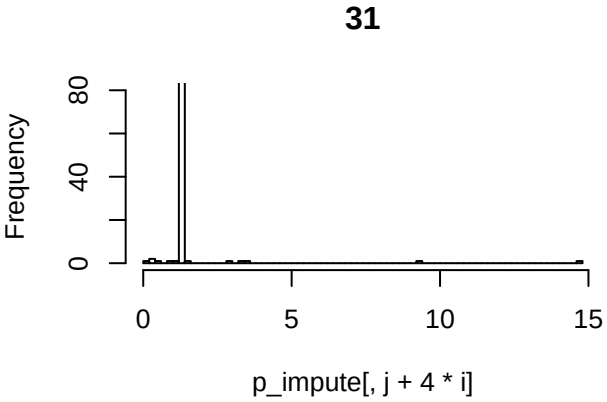

27
Frequency
0
40
80
0
5
10
15
p_impute[, j + 4 * i]

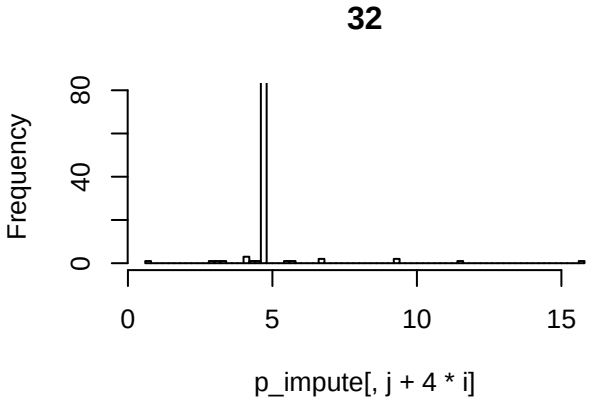

28
Frequency
0
40
80
4
5
6
7
8
9
p_impute[, j + 4 * i]

```
## [1] 6
```

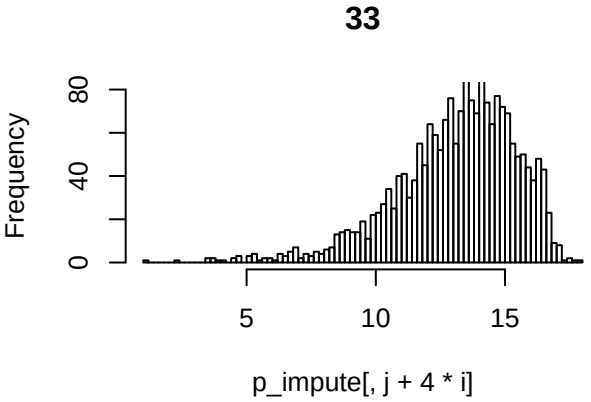

29
Frequency
0
40
80
2
3
4
5
6
7
8
p_impute[, j + 4 * i]

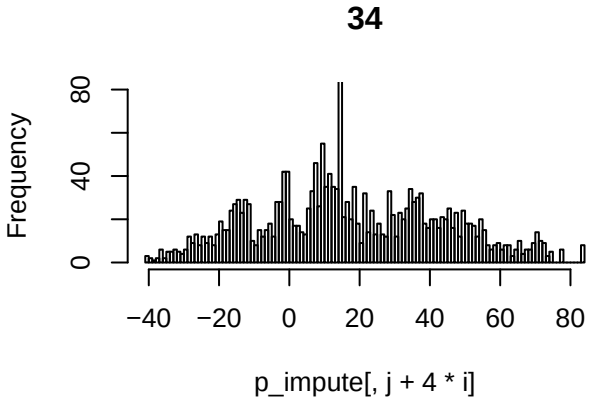

30
Frequency
0
40
80
1
2
3
4
5
p_impute[, j + 4 * i]

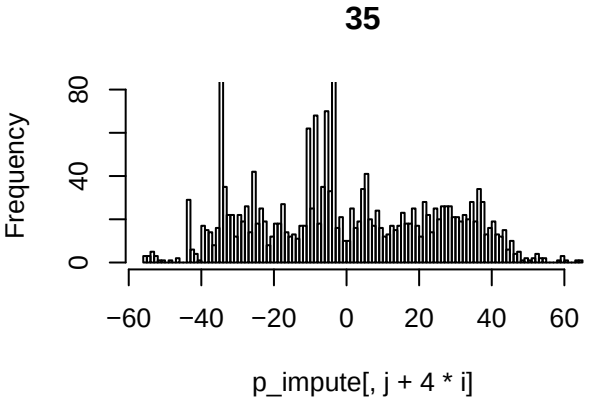

31
Frequency
0
40
80
0
5
10
15
p_impute[, j + 4 * i]

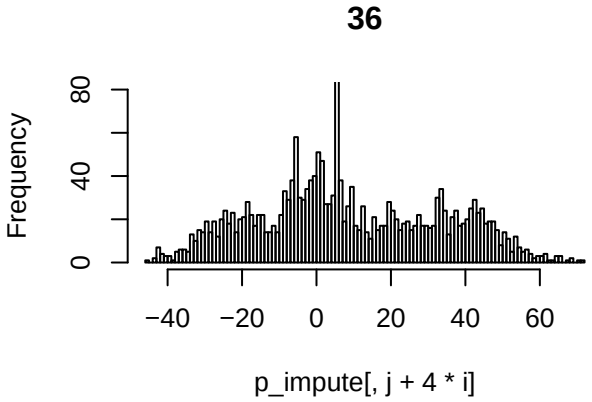

32
Frequency
0
40
80
0
5
10
15
p_impute[, j + 4 * i]

```
## [1] 7
```

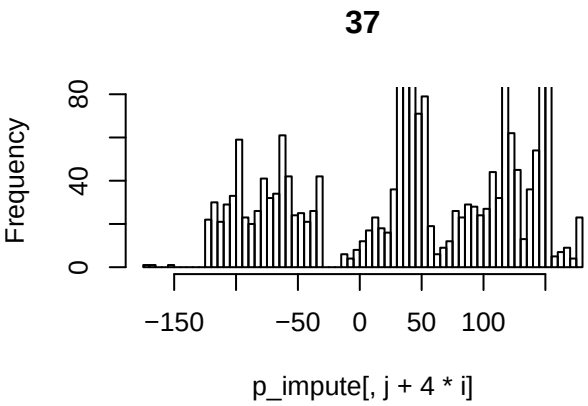

33
Frequency
0
40
80
5
10
15
p_impute[, j + 4 * i]

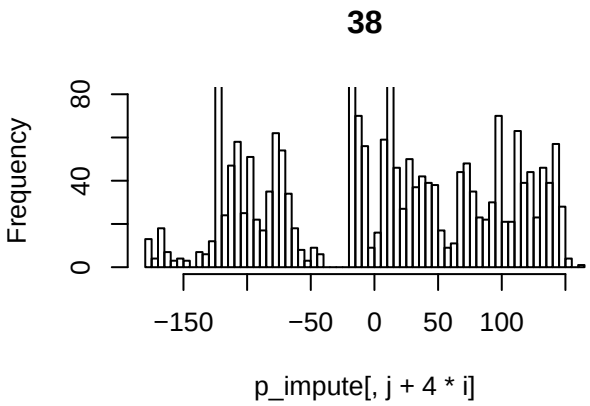

34
Frequency
0
40
80
−40
−20
0
20
40
60
80
p_impute[, j + 4 * i]

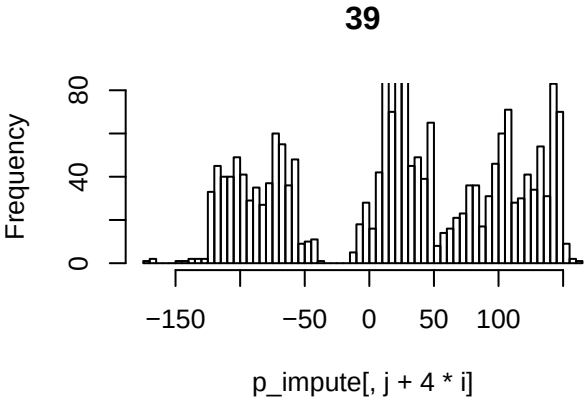

35
Frequency
0
40
80
−60
−40
−20
0
20
40
60
p_impute[, j + 4 * i]

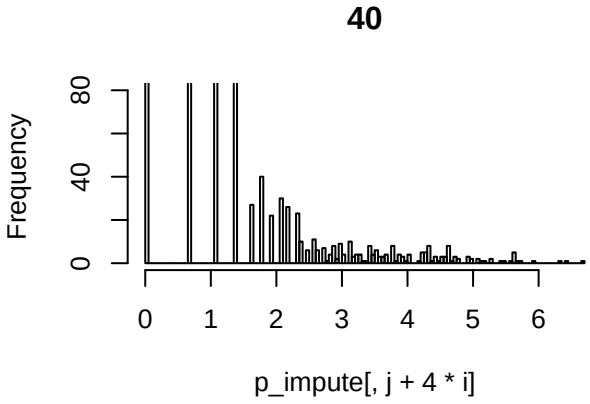

36
Frequency
0
40
80
−40
−20
0
20
40
60
p_impute[, j + 4 * i]

```
## [1] 8
```

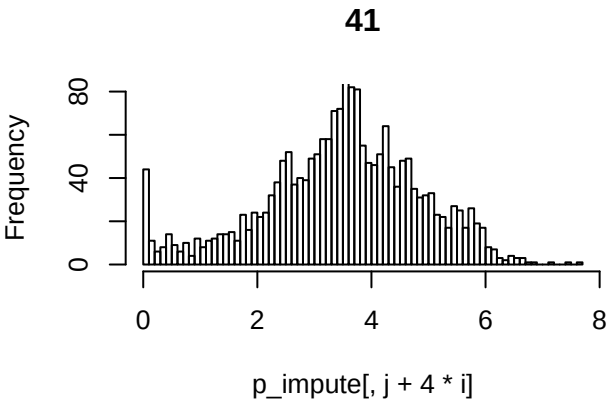

37
Frequency
0
40
80
−150
−50
0
50
100
p_impute[, j + 4 * i]

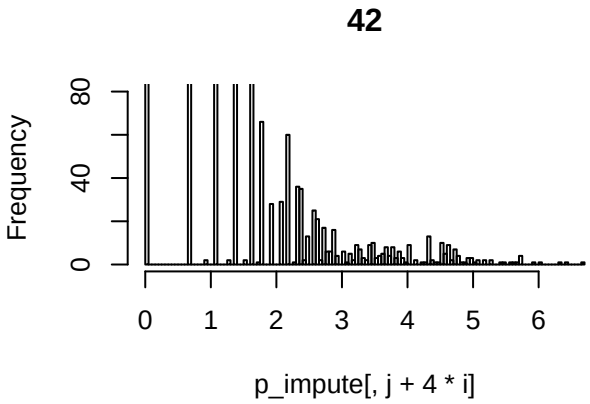

38
Frequency
0
40
80
−150
−50
0
50
100
p_impute[, j + 4 * i]

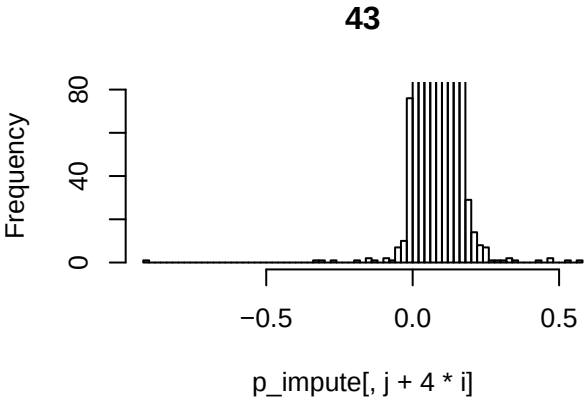

39
Frequency
0
40
80
−150
−50
0
50
100
p_impute[, j + 4 * i]

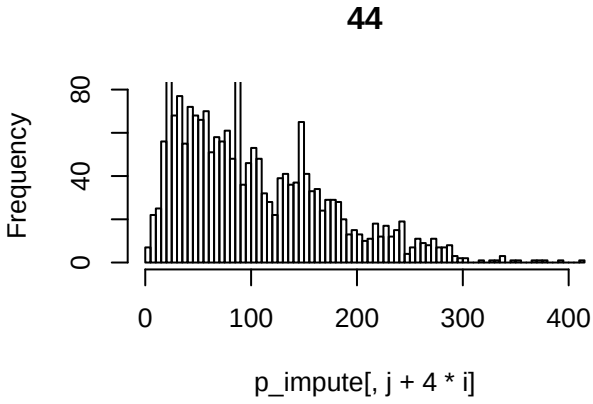

40
Frequency
0
40
80
0
1
2
3
4
5
6
p_impute[, j + 4 * i]

```
## [1] 9
```

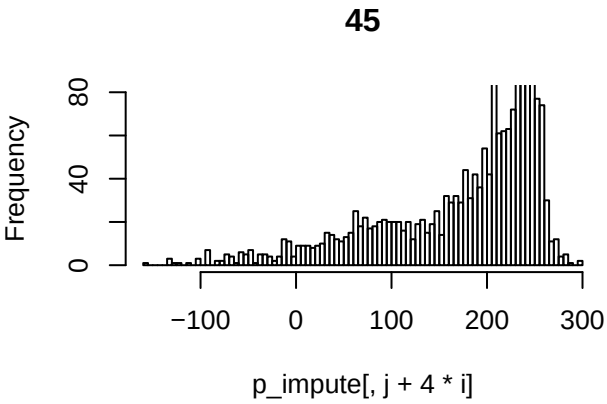

41
Frequency
0
40
80
0
2
4
6
8
p_impute[, j + 4 * i]

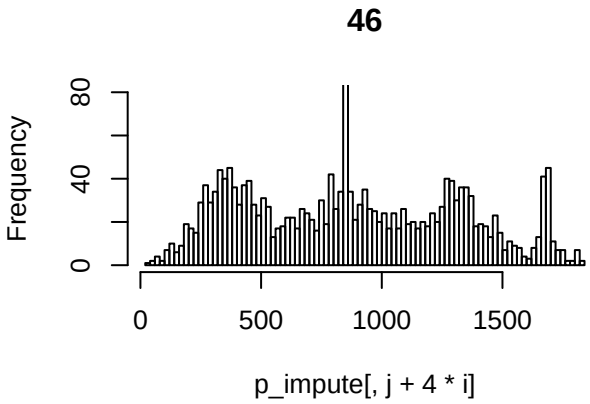

42
Frequency
0
40
80
0
1
2
3
4
5
6
p_impute[, j + 4 * i]

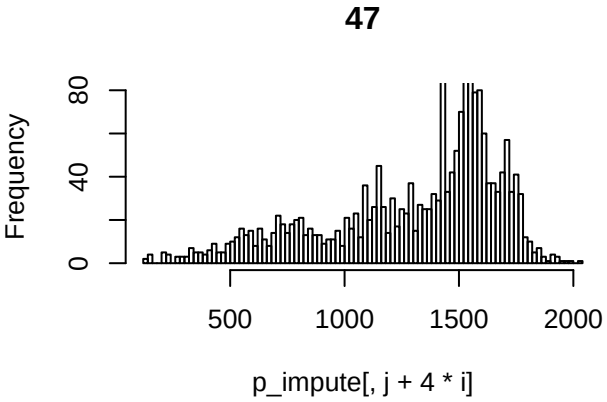

43
Frequency
0
40
80
−0.5
0.0
0.5
p_impute[, j + 4 * i]

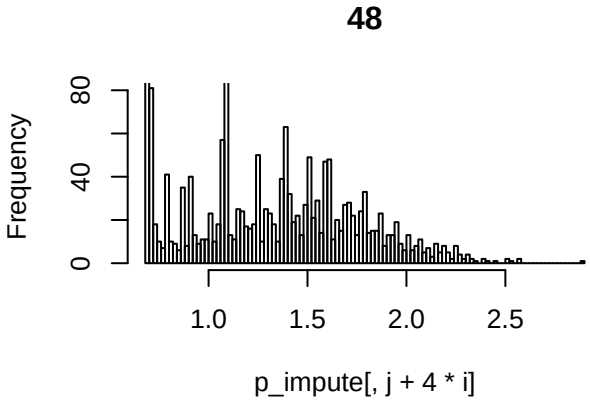

44
Frequency
0
40
80
0
100
200
300
400
p_impute[, j + 4 * i]

```
## [1] 10
```










```
## [1] 11
```

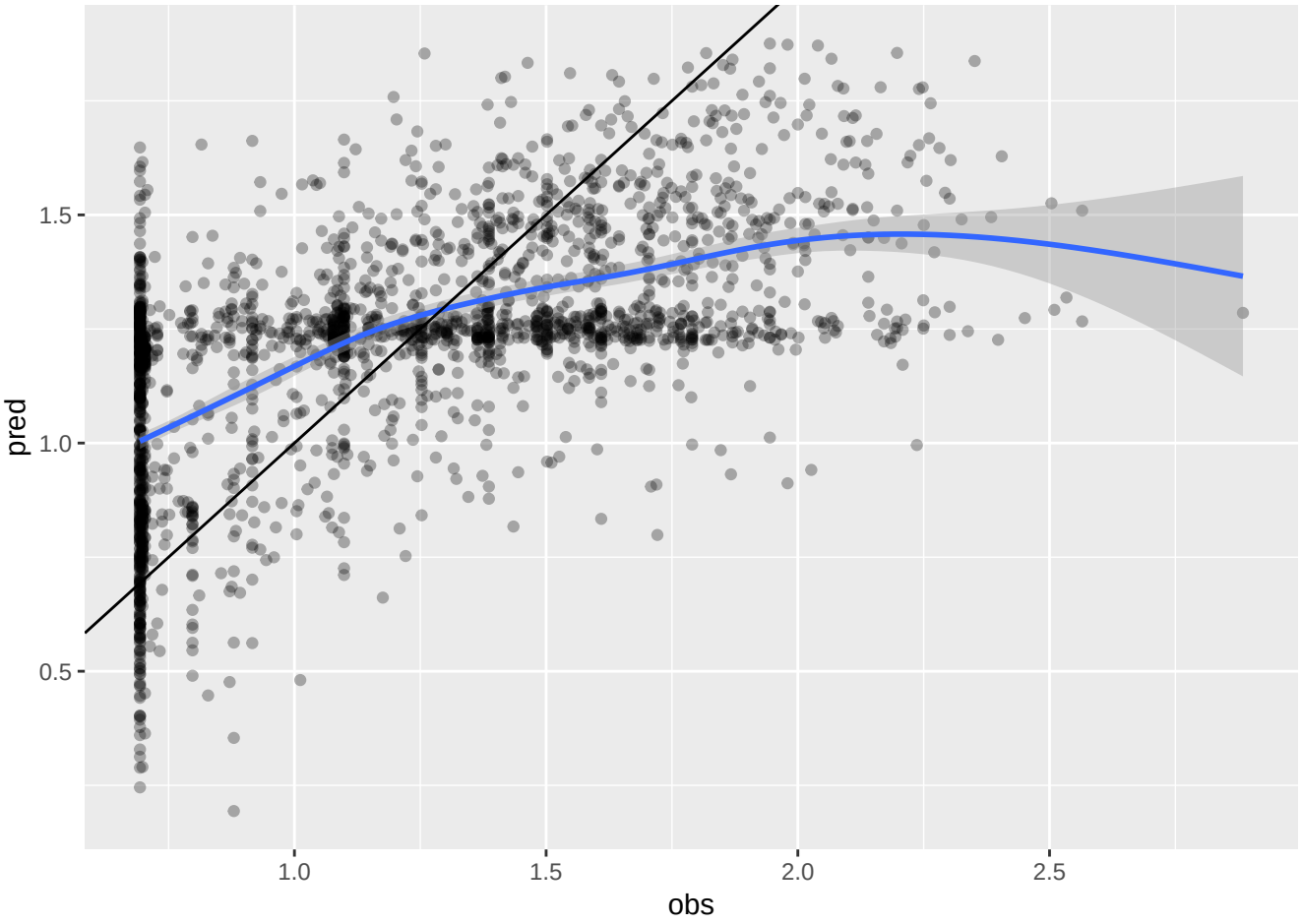
Now fit 4 models.

```
folds <- createFolds(p$y, k = 5, returnTrain = TRUE)
trcntrl <- trainControl(index = folds, savePredictions = TRUE, search = 'random')
```

```
cl <- makeForkCluster(6)
registerDoParallel(cl)
```

```
apriori_formula <- y ~ X5.1_AdultBodyMass_g + X3.1_AgeatFirstBirth_d + X18.1_BasalMetRate_mLO2hr + X9.1_Gestat
m0_lm <- train(apriori_formula, data = p_impute, method = 'lm', trControl = trcntrl, na.action = na.omit)

plotCV(m0_lm)
```

```
## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
```




```
m0_lm
```

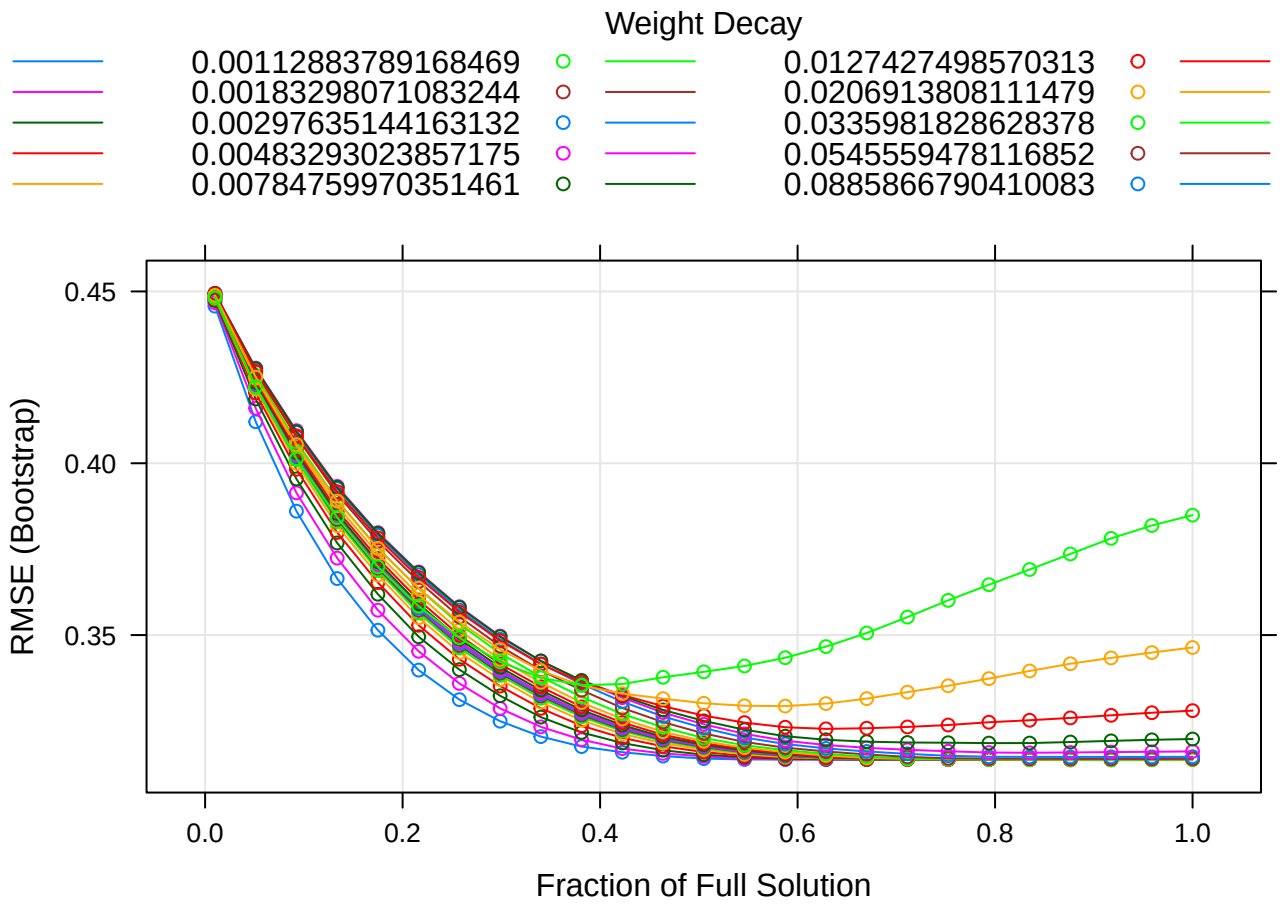
```
## Linear Regression
##
## 2143 samples
##    6 predictors
##
## No pre-processing
## Resampling: Bootstrapped (5 reps)
## Summary of sample sizes: 1714, 1715, 1714, 1715, 1714
## Resampling results:
##
##   RMSE       Rsquared  MAE
##   0.3705782  0.337926  0.2967044
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

```
summary(m0_lm$finalModel)
```

```
##
## Call:
## lm(formula = .outcome ~ ., data = dat)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.92083 -0.24850 -0.01827  0.23556  1.59271
##
## Coefficients:
##                             Estimate Std. Error t value Pr(>|t|)
## (Intercept)                2.897e+00  9.188e-02  31.535  < 2e-16 ***
## X5.1_AdultBodyMass_g      -1.732e-02  3.739e-03  -4.632 3.83e-06 ***
```

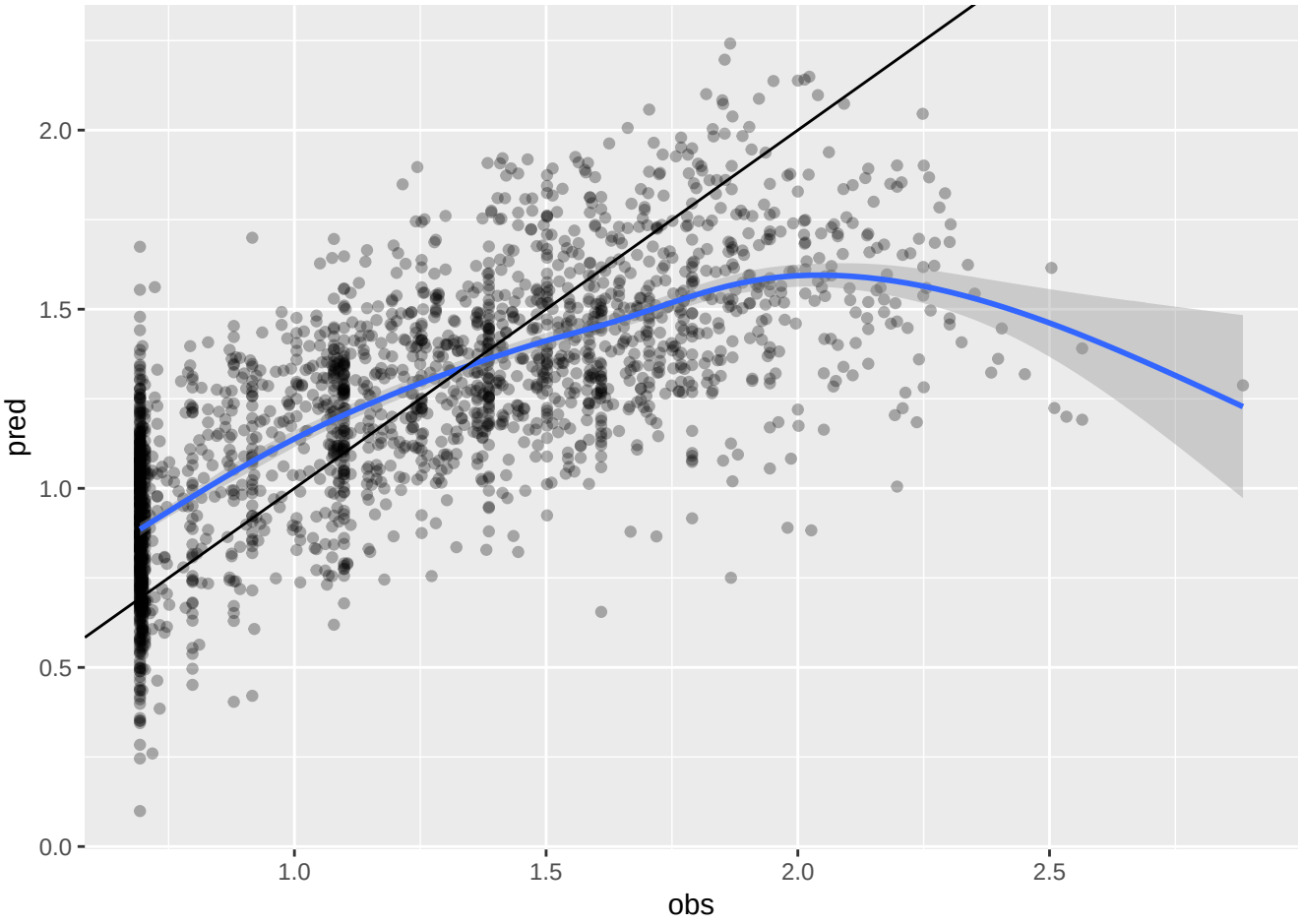
```
## X3.1_AgeatFirstBirth_d     6.012e-06  2.455e-05   0.245   0.8066
## X18.1_BasalMetRate_mLO2hr  1.368e-02  9.846e-03   1.389   0.1648
## X9.1_GestationLen_d       -2.710e-01  1.574e-02 -17.214  < 2e-16 ***
## X16.1_LittersPerYear       1.548e-02  9.368e-03   1.652   0.0987 .
## X17.1_MaxLongevity_m      -1.082e-01  1.624e-02  -6.662 3.42e-11 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.3704 on 2136 degrees of freedom
## Multiple R-squared:  0.3402, Adjusted R-squared:  0.3383
## F-statistic: 183.5 on 6 and 2136 DF,  p-value: < 2.2e-16
```

```
enet_gr <- expand.grid(lambda = 10 ^ seq(0, -4, length.out = 20), fraction = c(seq(0.01, 1, length.out = 25)))
m1_enet <- train(y ~ ., data = p_impute, method = 'enet', tuneGrid = enet_gr, trControl = trcntrl, na.action =

plot(m1_enet)
```




```
plotCV(m1_enet)
```

```
## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
```

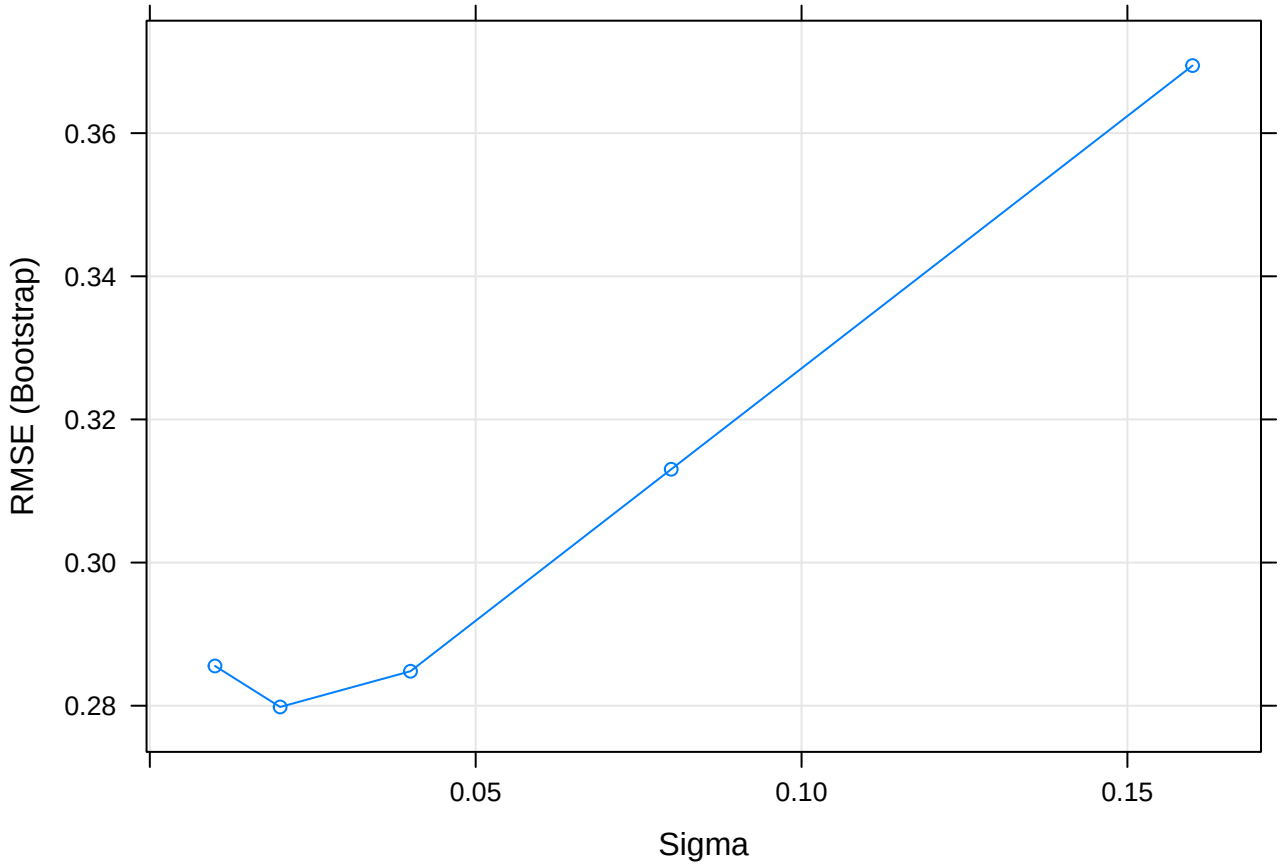



```
m1_enet$results$Rsquared %>% max
```

```
## [1] 0.526839
```

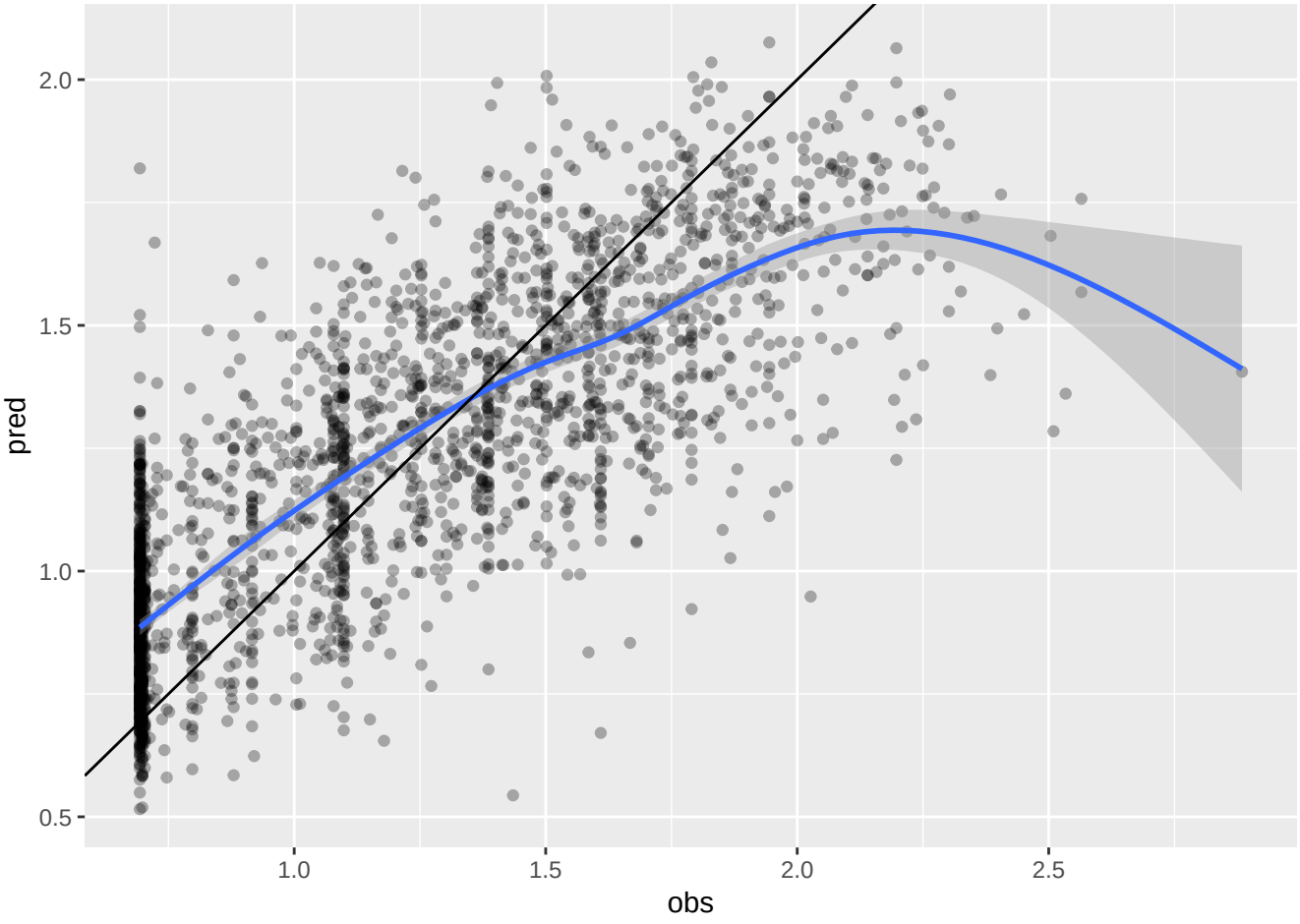
```
# Find the final parameters
#   https://stackoverflow.com/questions/40088228/how-to-retrieve-elastic-net-coefficients
#final_pars <- predict.enet(m1_enet$finalModel, s=m1_enet$bestTune[1, "fraction"], type="coef", mode="fraction
#final_pars
#sum(final_pars != 0)
```

```
gp_gr <- data.frame(sigma = c(0.01, 0.02, 0.04, 0.08, 0.16))
m2_gp <- train(y ~ ., data = p_impute, method = 'gaussprRadial', tuneGrid = gp_gr, trControl = trcntrl, na.act

plot(m2_gp)
```




```
plotCV(m2_gp)
```

```
## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
```



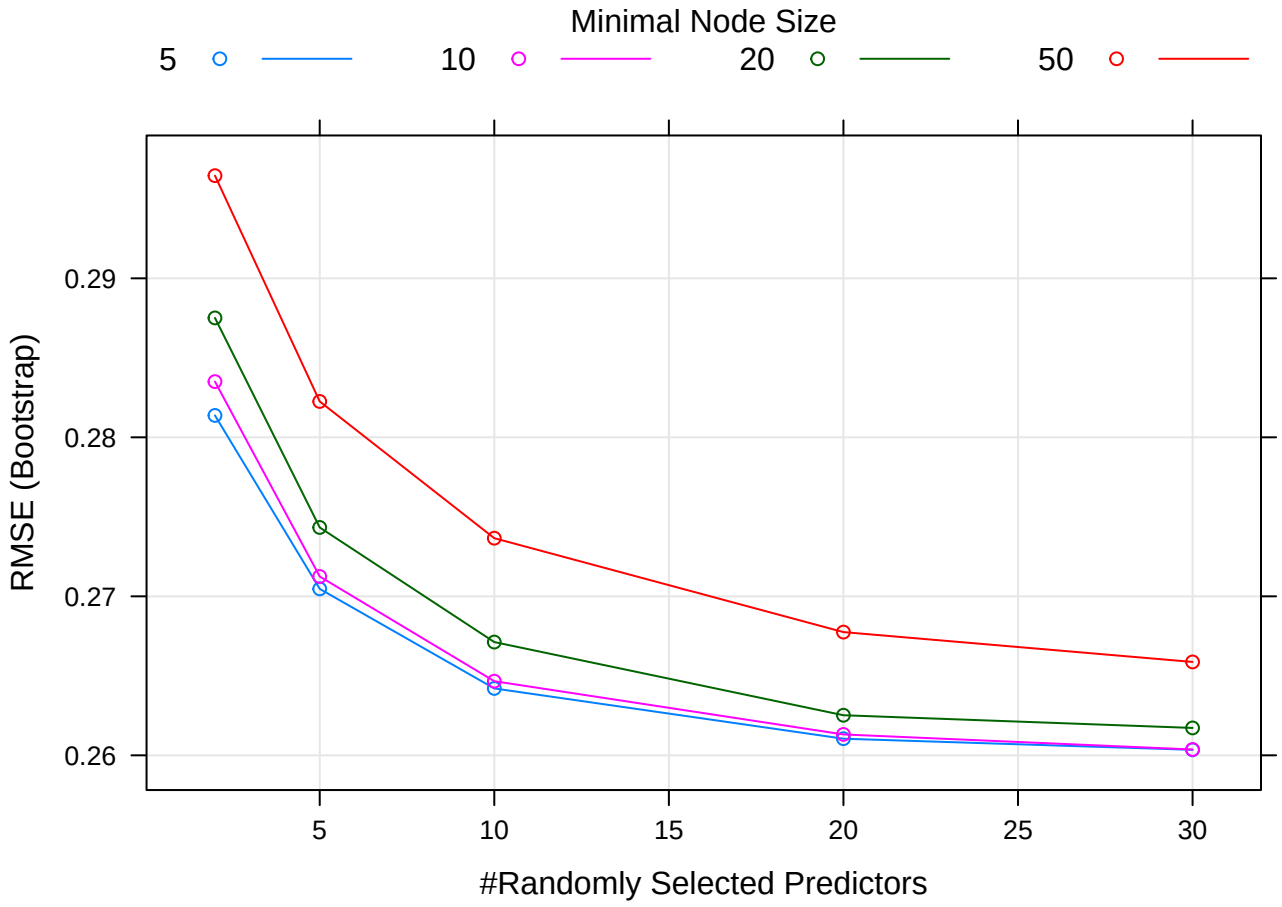
```
m2_gp
```

```
## Gaussian Process with Radial Basis Function Kernel
##
## 2143 samples
##   47 predictors
##
## No pre-processing
## Resampling: Bootstrapped (5 reps)
## Summary of sample sizes: 1714, 1715, 1714, 1715, 1714
## Resampling results across tuning parameters:
##
##   sigma  RMSE       Rsquared   MAE
##   0.01   0.2855551  0.6095879  0.2218111
##   0.02   0.2798232  0.6266082  0.2183842
##   0.04   0.2848164  0.6178132  0.2253383
##   0.08   0.3130373  0.5515241  0.2540034
##   0.16   0.3694406  0.3992555  0.3080410
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was sigma = 0.02.
```

```
m2_gp$results$Rsquared %>% max
```

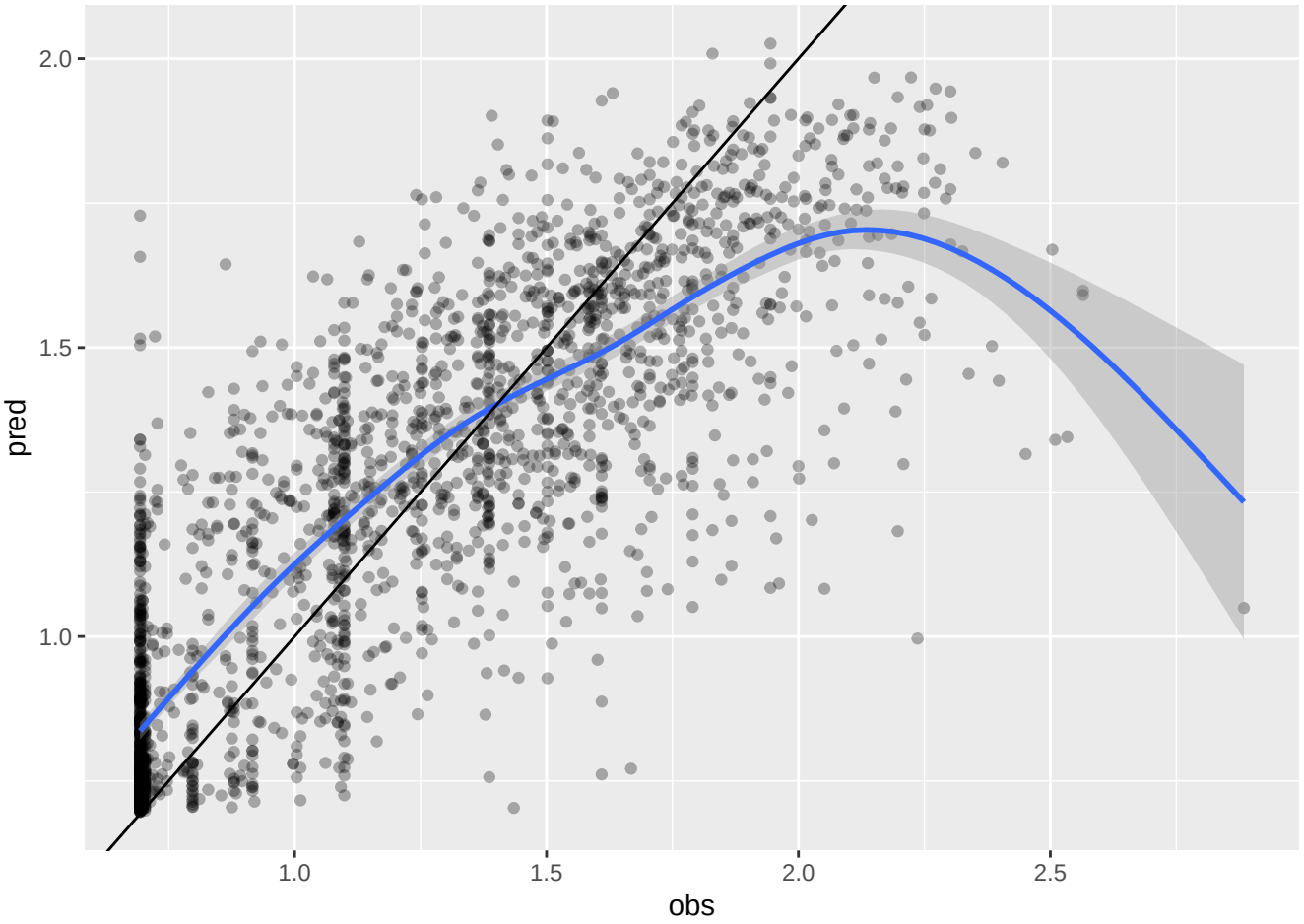
```
## [1] 0.6266082
```

```
rf_gr <- expand.grid(mtry = c(2, 5, 10, 20, 30), splitrule = 'variance', min.node.size = c(5, 10, 20, 50))
m3_rf <- train(y ~ ., data = p_impute, method = 'ranger', tuneGrid = rf_gr, trControl = trcntrl, na.action = n

plot(m3_rf)
```




```
plotCV(m3_rf)
```

```
## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
```




```
m3_rf
```

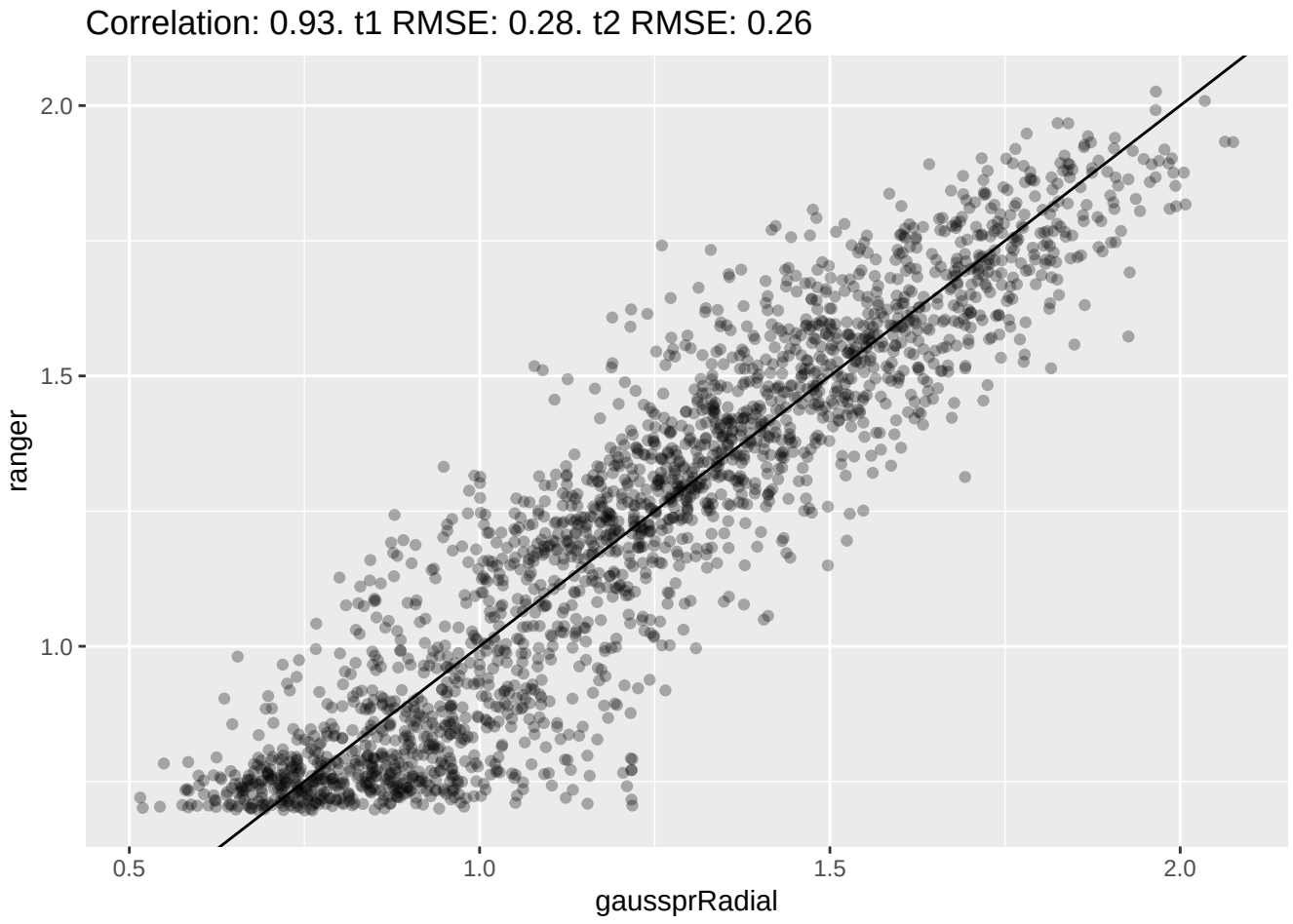
```
## Random Forest
##
## 2143 samples
##   47 predictors
##
## No pre-processing
## Resampling: Bootstrapped (5 reps)
## Summary of sample sizes: 1714, 1715, 1714, 1715, 1714
## Resampling results across tuning parameters:
##
##   mtry  min.node.size  RMSE       Rsquared   MAE
##    2     5             0.2813761  0.6405606  0.2177796
##    2    10             0.2835044  0.6354284  0.2200403
##    2    20             0.2875085  0.6262929  0.2241080
##    2    50             0.2964571  0.6058430  0.2331574
##    5     5             0.2704681  0.6595899  0.2051341
##    5    10             0.2712469  0.6583178  0.2062279
##    5    20             0.2743309  0.6517933  0.2096598
##    5    50             0.2822554  0.6332837  0.2178622
##   10     5             0.2642059  0.6711550  0.1980803
##   10    10             0.2646623  0.6705596  0.1986097
##   10    20             0.2671232  0.6649359  0.2013062
##   10    50             0.2736562  0.6499851  0.2081583
##   20     5             0.2610452  0.6756351  0.1930300
##   20    10             0.2613128  0.6751686  0.1935159
##   20    20             0.2625209  0.6725189  0.1952154
##   20    50             0.2677504  0.6604168  0.2009672
```

```
##    30     5             0.2603446  0.6761010  0.1913242
##    30    10             0.2603651  0.6761785  0.1915433
##    30    20             0.2617231  0.6728620  0.1931893
##    30    50             0.2658725  0.6631516  0.1981692
##
## Tuning parameter 'splitrule' was held constant at a value of variance
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were mtry = 30, splitrule =
##  variance and min.node.size = 5.
```

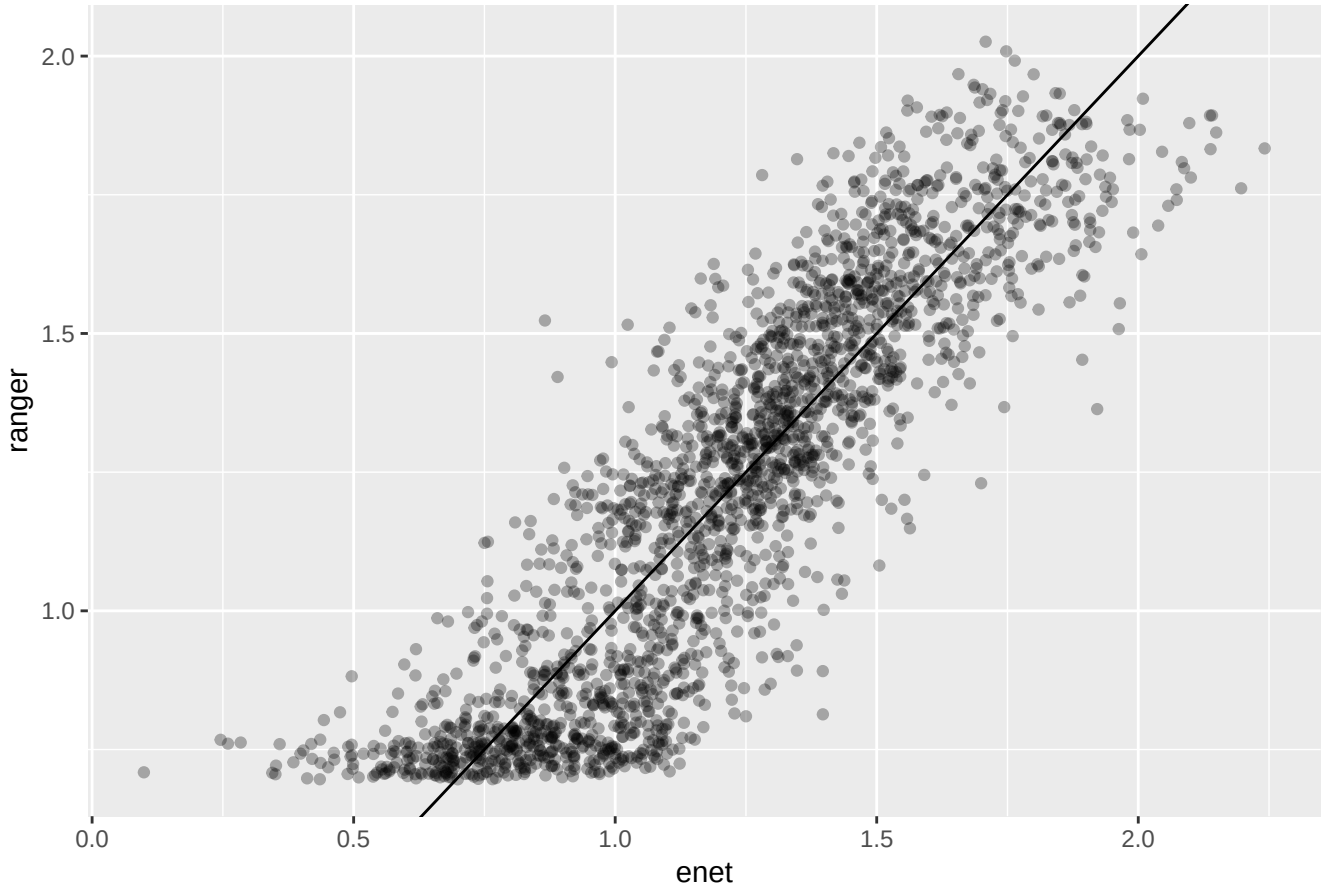
```
m3_rf$results$Rsquared %>% max
```

```
## [1] 0.6761785
```

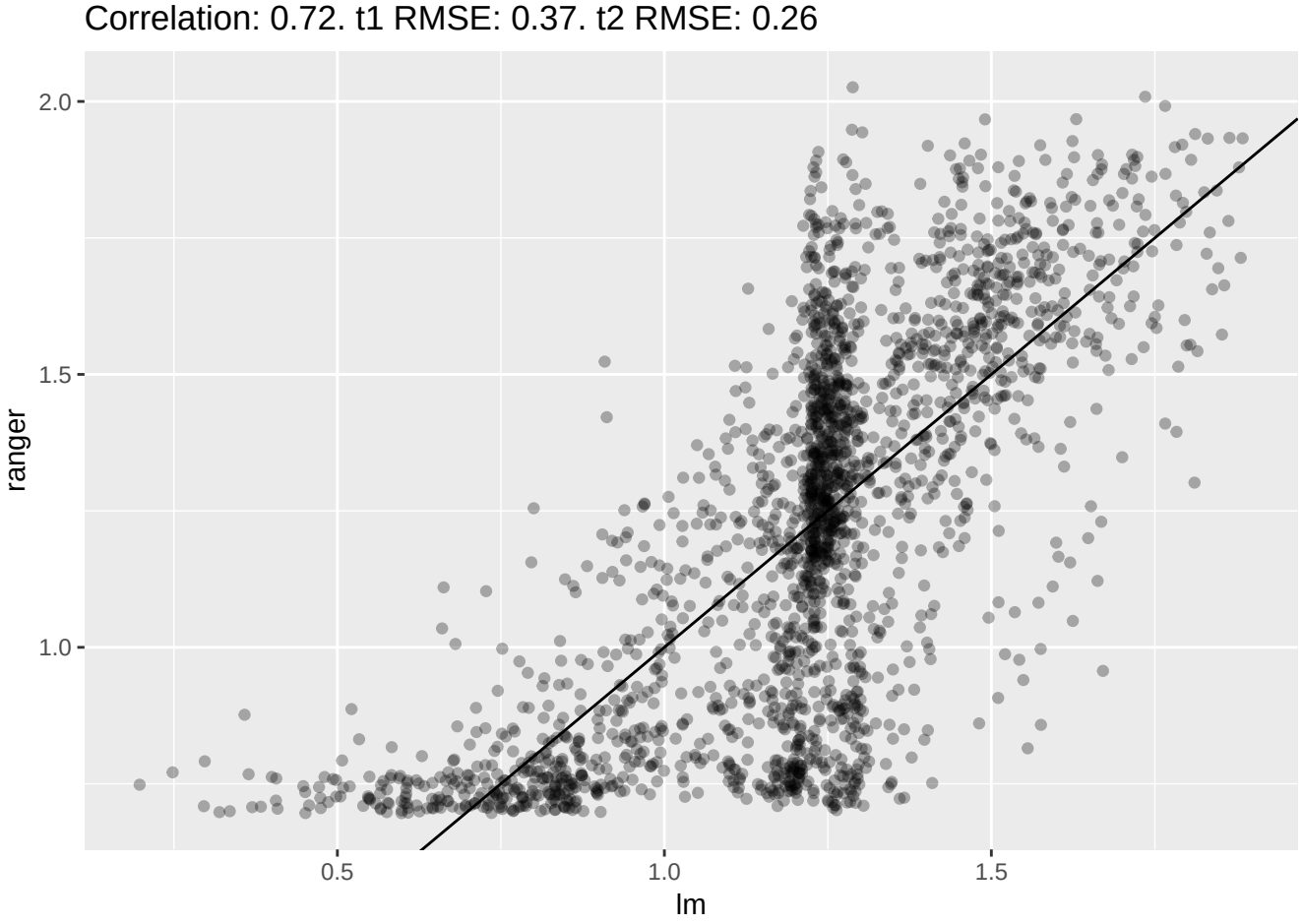
```
compare_models(m2_gp, m3_rf)
```




```
compare_models(m1_enet, m3_rf)
```




```
compare_models(m0_lm, m3_rf)
```



Global analysis.

- gain some understanding of a system
  - predictability
  - complexity
  - r2 # Generate hypotheses to test more formally.
- generate hypotheses (variable level)
  - var imp
  - interaction importance
  - ice etc. # Find variable importance for each model

```
varImp(m1_enet)
```

```
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric =
## parametric, : zero-width neighborhood. make span bigger

## Warning in simpleLoess(y, x, w, span, degree = degree, parametric =
## parametric, : pseudoinverse used at 4.8037

## Warning in simpleLoess(y, x, w, span, degree = degree, parametric =
## parametric, : neighborhood radius 0.0031927

## Warning in simpleLoess(y, x, w, span, degree = degree, parametric =
## parametric, : reciprocal condition number 0

## loess r-squared variable importance
##
##   only 20 most important variables shown (out of 47)
##
##                               Overall
## X9.1_GestationLen_d            100.00
## X5.1_AdultBodyMass_g            70.67
```

```
## X26.4_GR_MidRangeLat_dd         67.42
## X26.3_GR_MinLat_dd              62.73
## X30.2_PET_Mean_mm               61.68
## X26.2_GR_MaxLat_dd              59.09
## X30.1_AET_Mean_mm               56.67
## X23.1_SexualMaturityAge_d       54.73
## X28.2_Temp_Mean_01degC          53.08
## X25.1_WeaningAge_d              52.97
## X17.1_MaxLongevity_m            51.87
## X13.1_AdultHeadBodyLen_mm       51.01
## X28.1_Precip_Mean_mm            49.70
## X5.3_NeonateBodyMass_g          45.56
## X21.1_PopulationDensity_n.km2   39.86
## X5.4_WeaningBodyMass_g          24.52
## X12.2_Terrestriality            23.43
## X26.7_GR_MidRangeLong_dd        23.14
## X26.6_GR_MinLong_dd             21.45
## X3.1_AgeatFirstBirth_d          20.41
```

```
varImp(m2_gp)
```

```
## Warning in simpleLoess(y, x, w, span, degree = degree, parametric =
## parametric, : zero-width neighborhood. make span bigger

## Warning in simpleLoess(y, x, w, span, degree = degree, parametric =
## parametric, : pseudoinverse used at 4.8037

## Warning in simpleLoess(y, x, w, span, degree = degree, parametric =
## parametric, : neighborhood radius 0.0031927

## Warning in simpleLoess(y, x, w, span, degree = degree, parametric =
## parametric, : reciprocal condition number 0

## loess r-squared variable importance
##
##   only 20 most important variables shown (out of 47)
##
##                                Overall
## X9.1_GestationLen_d             100.00
## X5.1_AdultBodyMass_g             70.67
## X26.4_GR_MidRangeLat_dd          67.42
## X26.3_GR_MinLat_dd               62.73
## X30.2_PET_Mean_mm                61.68
## X26.2_GR_MaxLat_dd               59.09
## X30.1_AET_Mean_mm                56.67
## X23.1_SexualMaturityAge_d        54.73
## X28.2_Temp_Mean_01degC           53.08
## X25.1_WeaningAge_d               52.97
## X17.1_MaxLongevity_m             51.87
## X13.1_AdultHeadBodyLen_mm        51.01
## X28.1_Precip_Mean_mm             49.70
## X5.3_NeonateBodyMass_g           45.56
## X21.1_PopulationDensity_n.km2    39.86
## X5.4_WeaningBodyMass_g           24.52
## X12.2_Terrestriality             23.43
## X26.7_GR_MidRangeLong_dd         23.14
## X26.6_GR_MinLong_dd              21.45
## X3.1_AgeatFirstBirth_d           20.41
```

```
varImp(m3_rf)
```

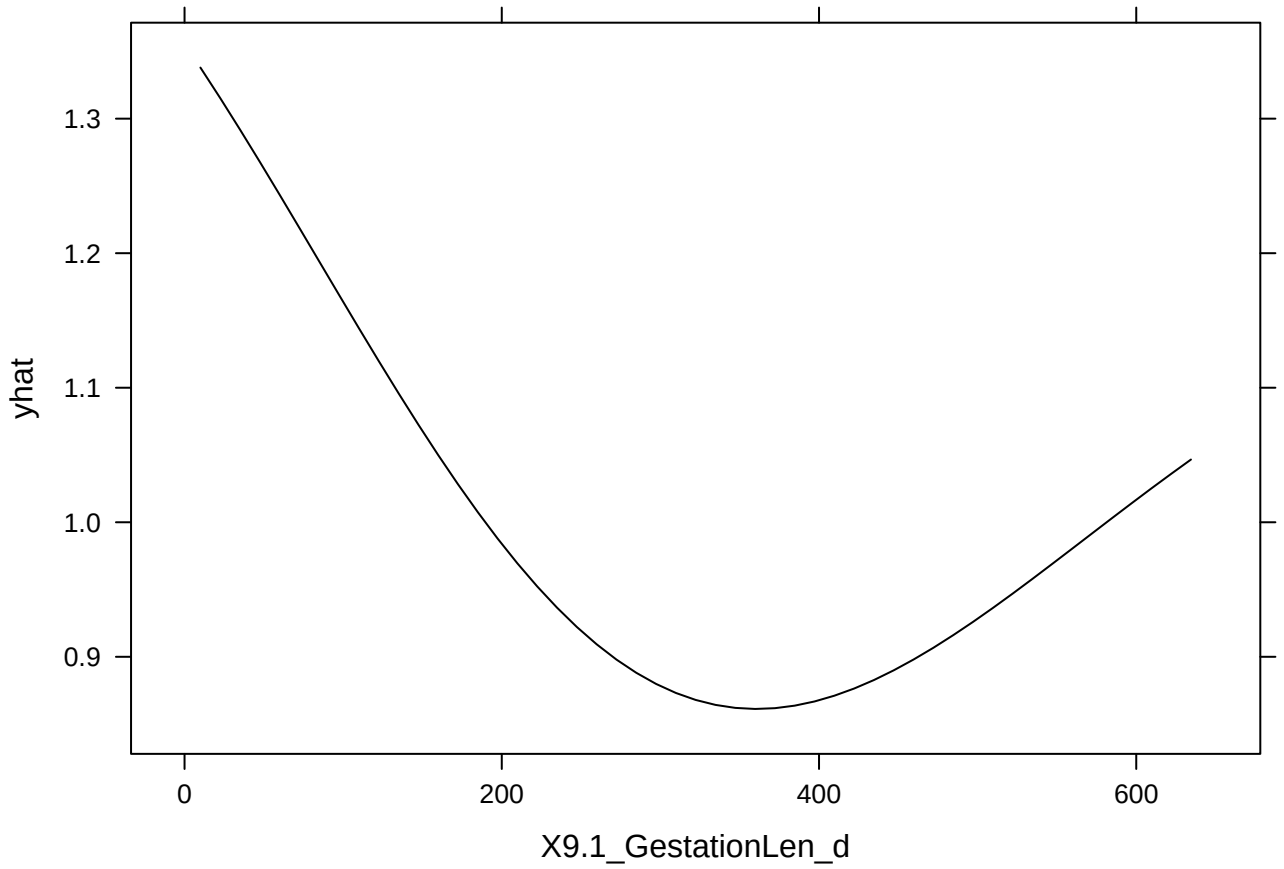
```
## ranger variable importance
##
```

```
##   only 20 most important variables shown (out of 47)
##
##                            Overall
## X9.1_GestationLen_d        100.000
## X5.1_AdultBodyMass_g        58.065
## X8.1_AdultForearmLen_mm     26.915
## X26.4_GR_MidRangeLat_dd     25.800
## X30.2_PET_Mean_mm           22.957
## X30.1_AET_Mean_mm           20.838
## X26.2_GR_MaxLat_dd          19.898
## X12.2_Terrestriality        15.658
## X26.1_GR_Area_km2           11.726
## X28.2_Temp_Mean_01degC      11.042
## X25.1_WeaningAge_d          10.726
## X12.1_HabitatBreadth        10.305
## X26.3_GR_MinLat_dd           9.542
## X28.1_Precip_Mean_mm         8.629
## X27.2_HuPopDen_Mean_n.km2    7.841
## X13.1_AdultHeadBodyLen_mm    7.649
## X17.1_MaxLongevity_m         7.229
## X23.1_SexualMaturityAge_d    7.223
## X26.6_GR_MinLong_dd          7.097
## X26.5_GR_MaxLong_dd          6.010
```

Now plot some functional forms

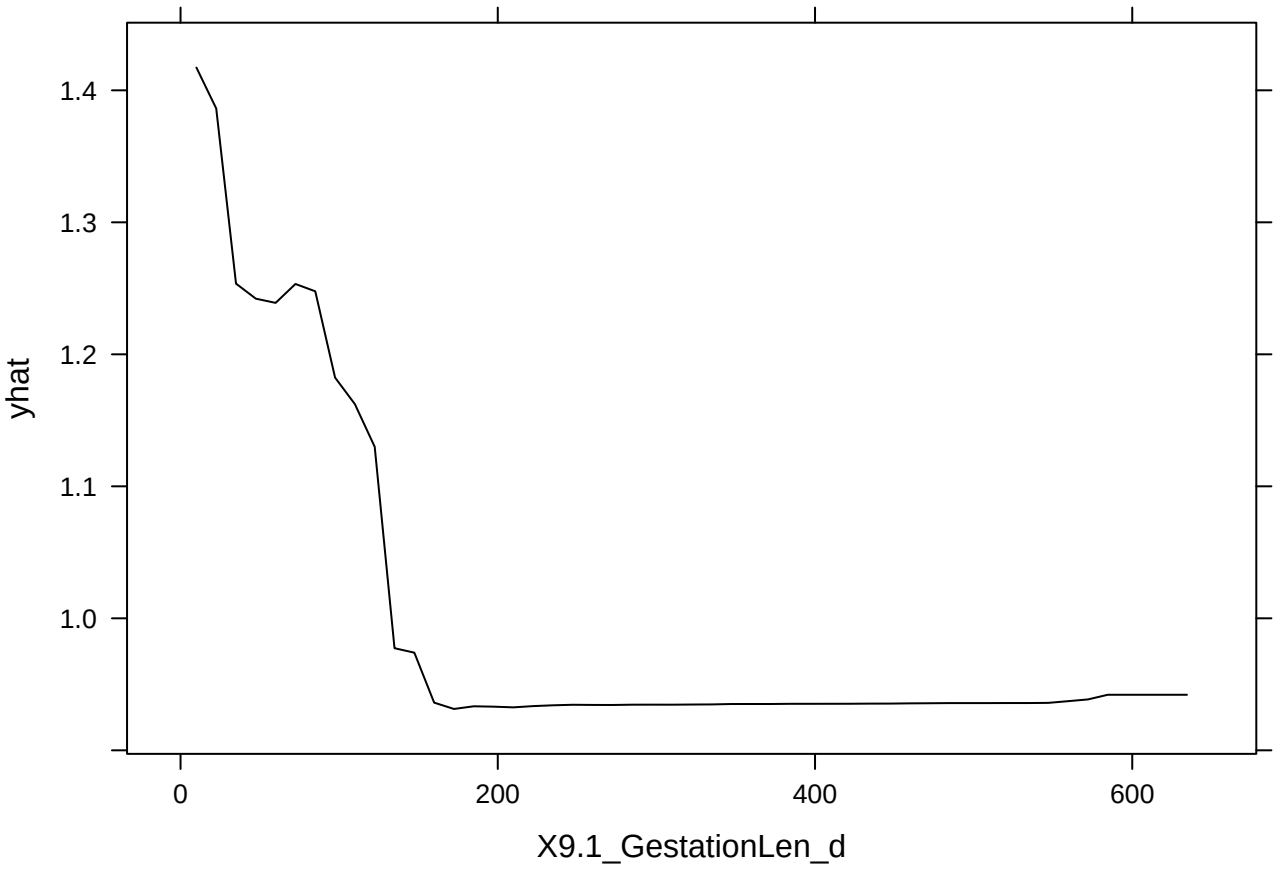
```
partial(m2_gp,
        pred.var = c('X9.1_GestationLen_d'),
        parallel = TRUE, plot = TRUE)
```

```
## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'

## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'
```



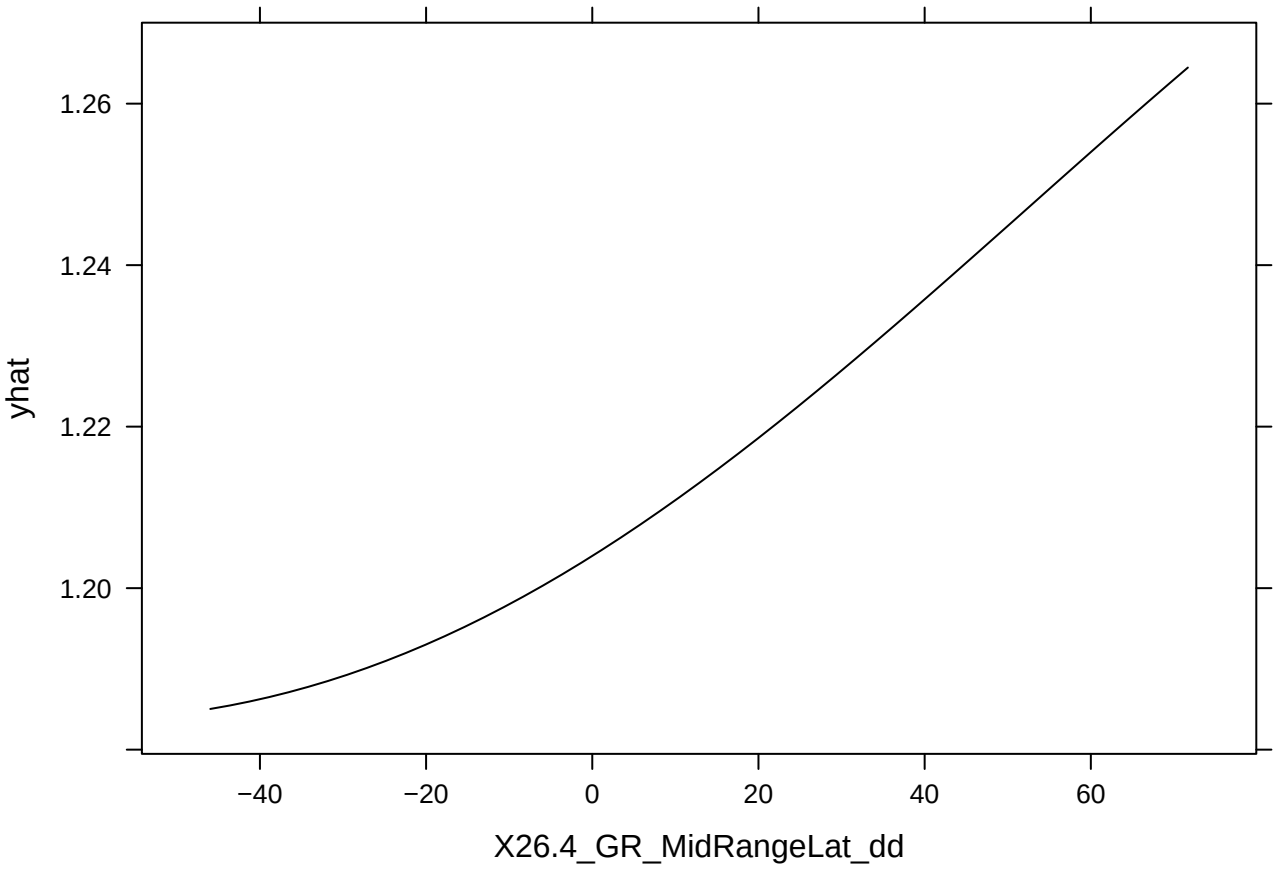

```
partial(m3_rf,
        pred.var = c('X9.1_GestationLen_d'),
        parallel = TRUE, plot = TRUE)
```

```
## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'

## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'
```



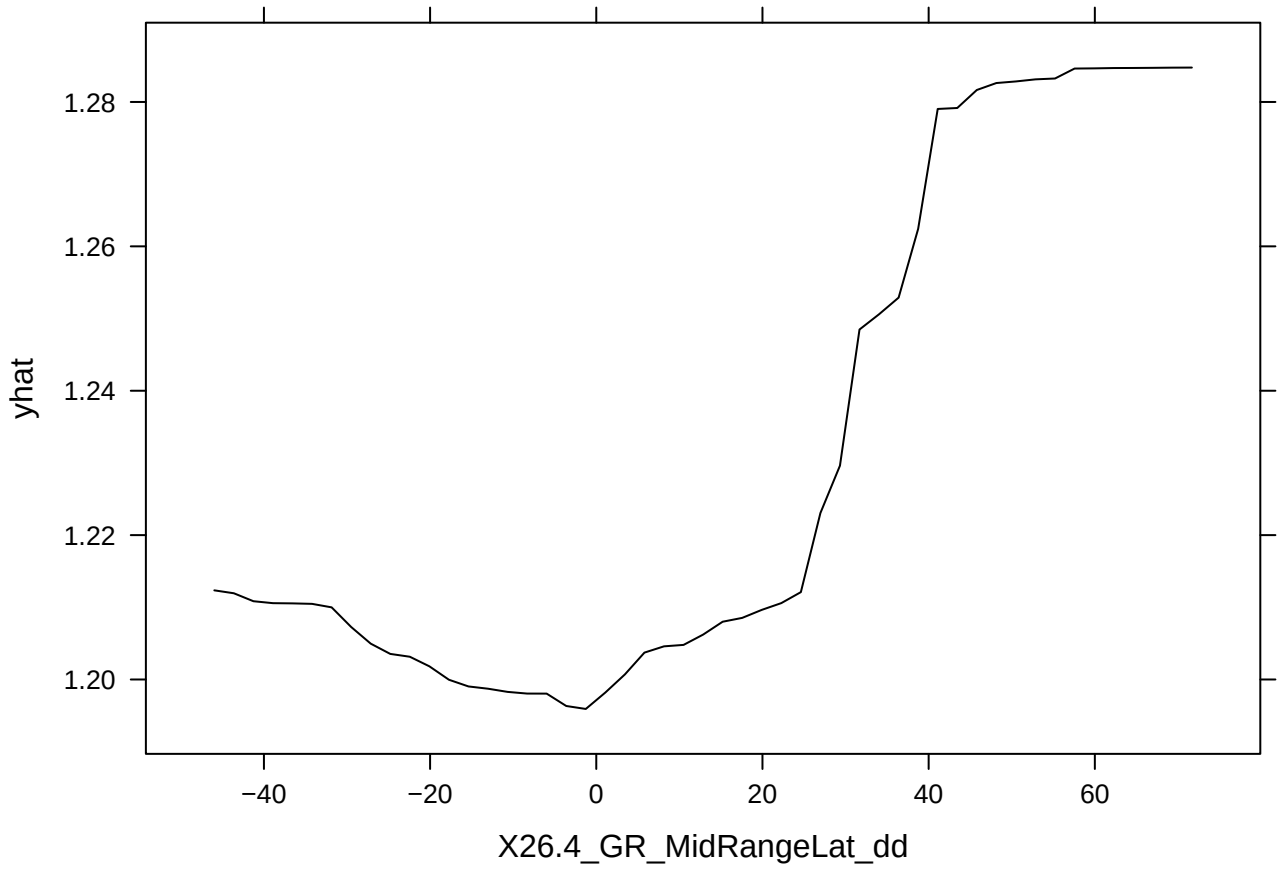

```
partial(m2_gp,
        pred.var = c('X26.4_GR_MidRangeLat_dd'),
        parallel = TRUE, plot = TRUE)
```

```
## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'

## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'
```



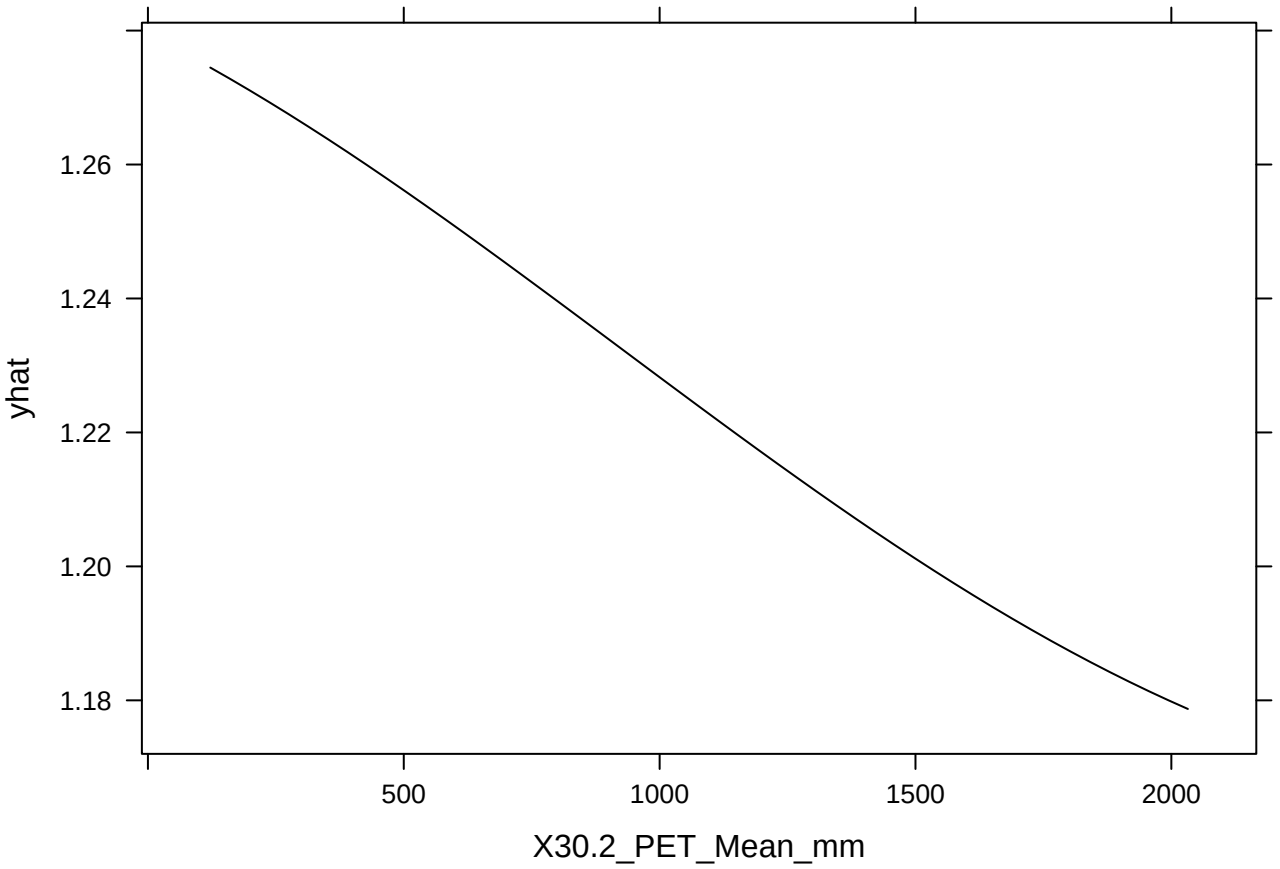

```
partial(m3_rf,
        pred.var = c('X26.4_GR_MidRangeLat_dd'),
        parallel = TRUE, plot = TRUE)
```

```
## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'

## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'
```



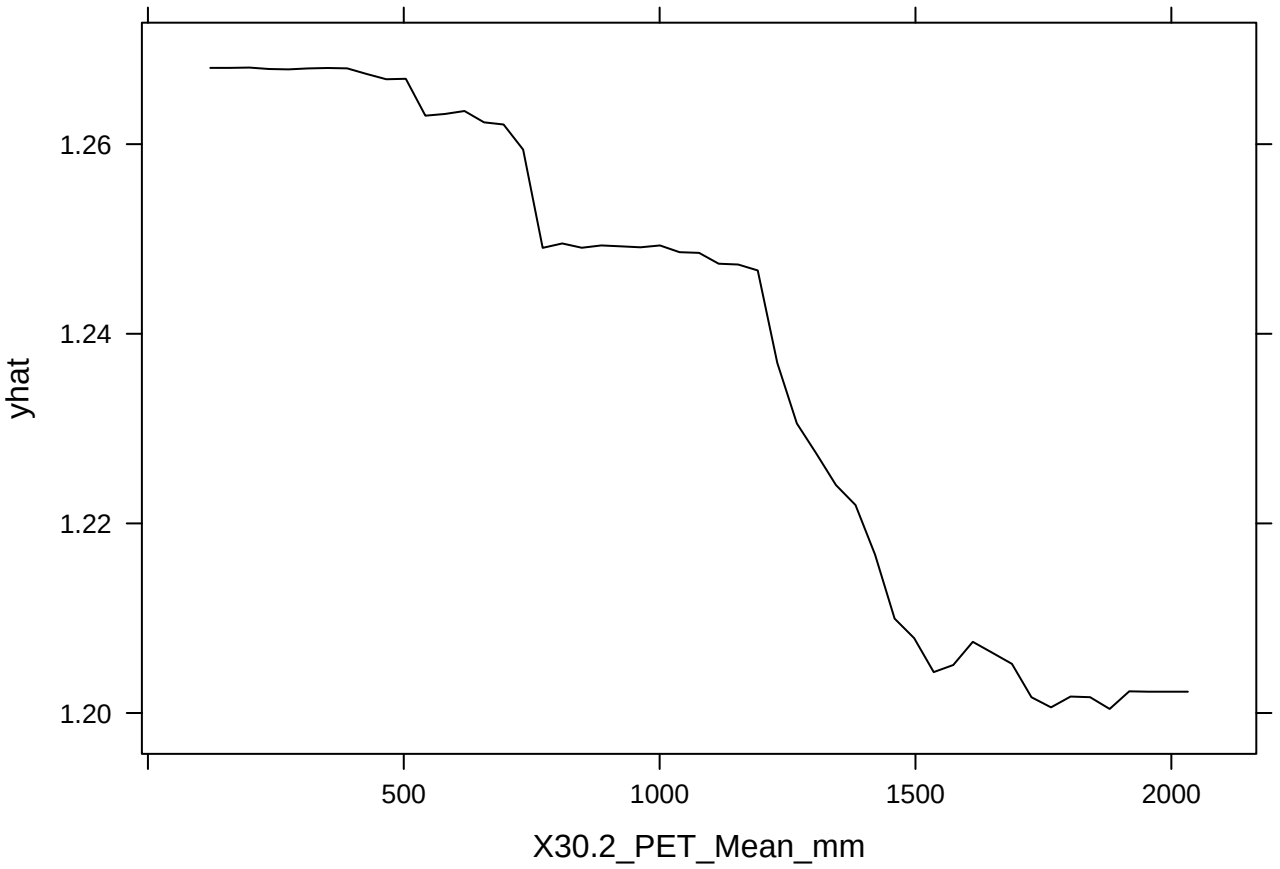

```
partial(m2_gp,
        pred.var = c('X30.2_PET_Mean_mm'),
        parallel = TRUE, plot = TRUE)
```

```
## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'

## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'
```



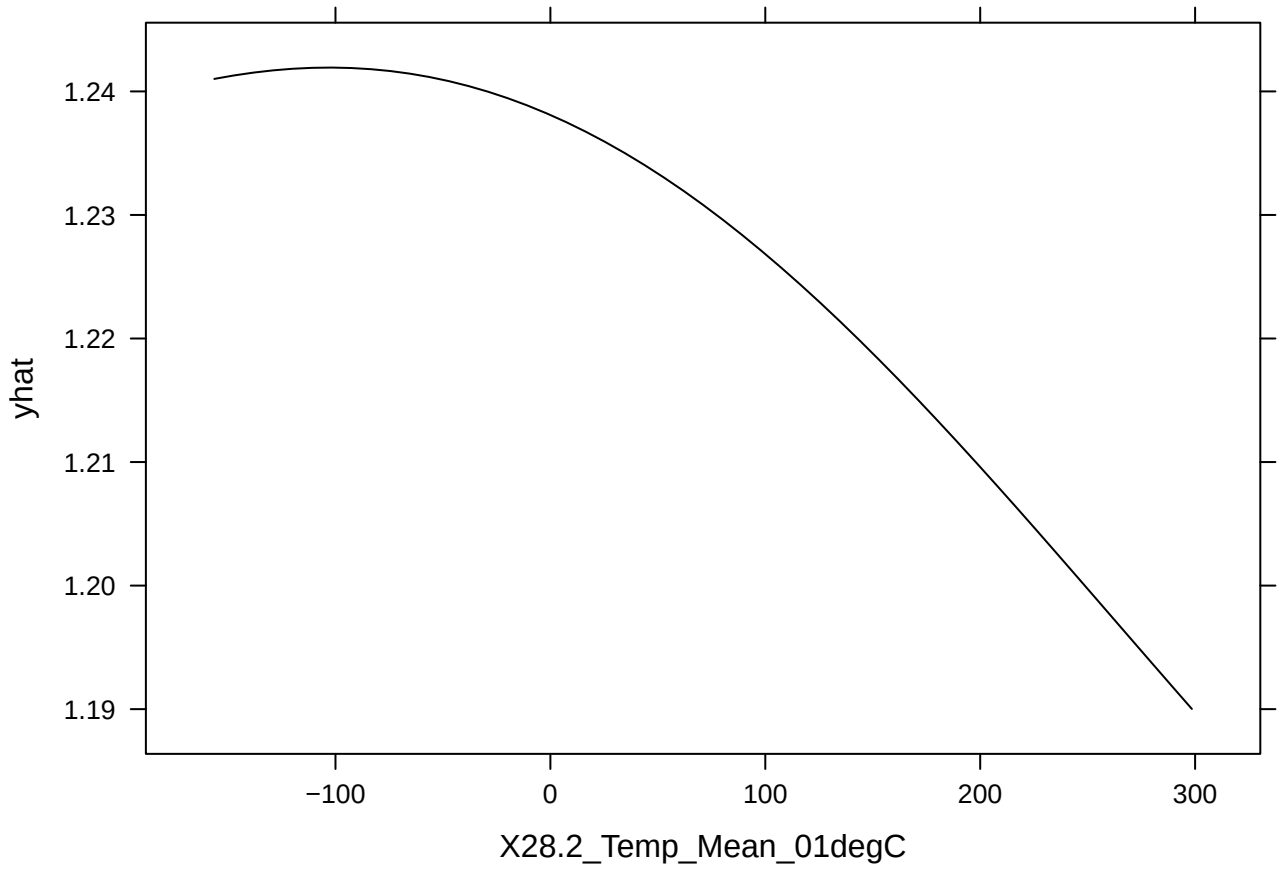

```
partial(m3_rf,
        pred.var = c('X30.2_PET_Mean_mm'),
        parallel = TRUE, plot = TRUE)
```

```
## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'

## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'
```



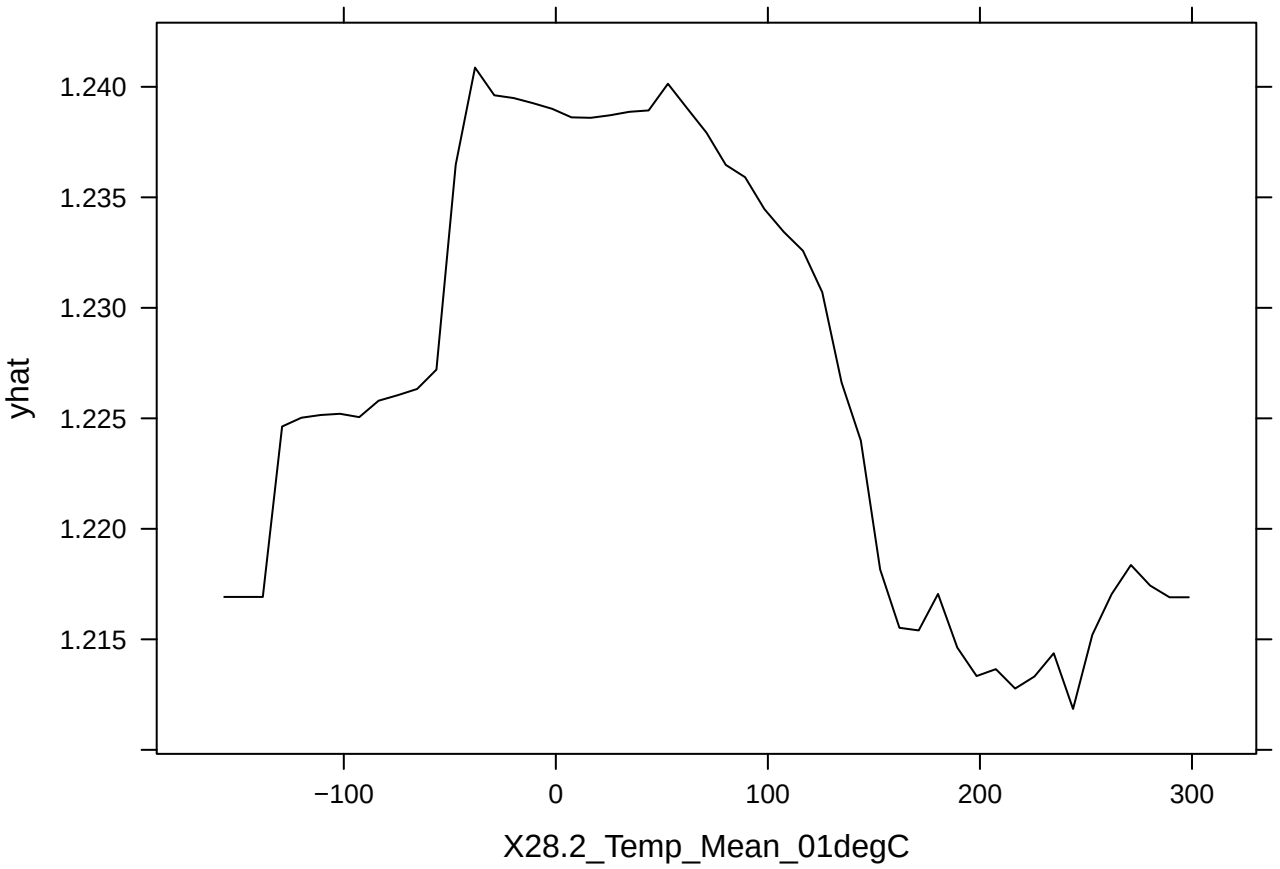

```
partial(m2_gp,
        pred.var = c('X28.2_Temp_Mean_01degC'),
        parallel = TRUE, plot = TRUE)
```

```
## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'

## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'
```



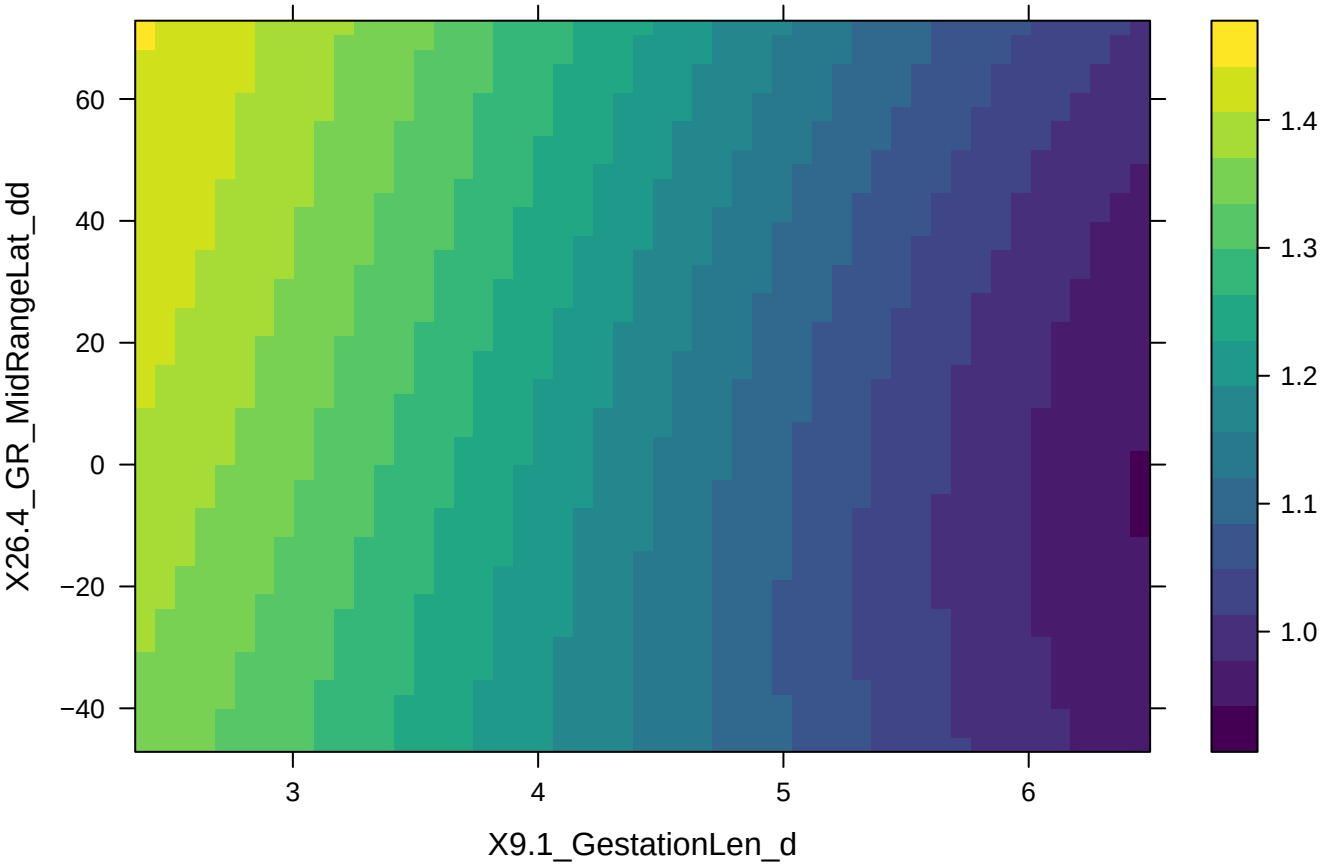

```
partial(m3_rf,
        pred.var = c('X28.2_Temp_Mean_01degC'),
        parallel = TRUE, plot = TRUE)
```

```
## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'

## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'
```



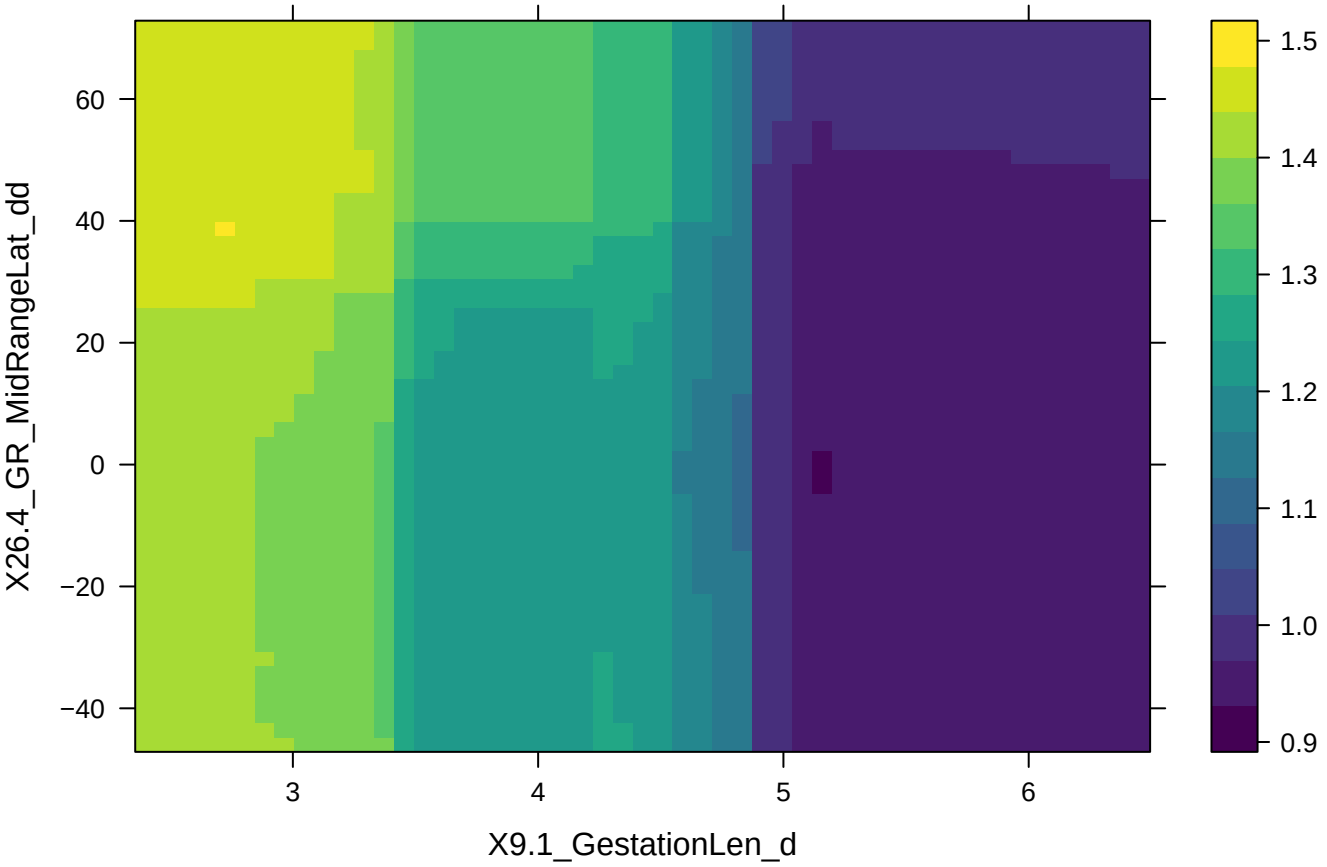

```
partial(m2_gp,
        pred.var = c('X9.1_GestationLen_d', 'X26.4_GR_MidRangeLat_dd'),
        parallel = TRUE, plot = TRUE)
```

```
## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'

## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'
```



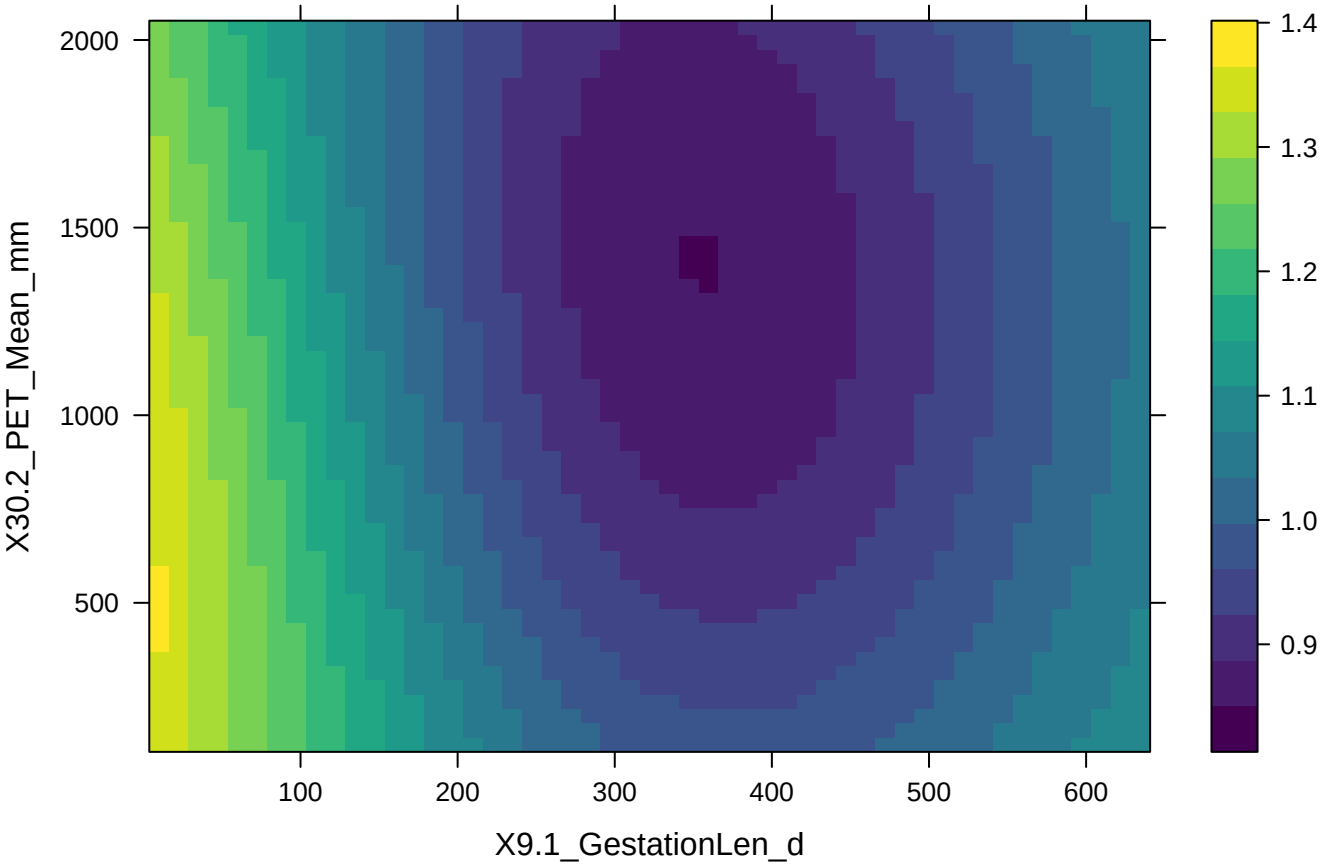

```
partial(m3_rf,
        pred.var = c('X9.1_GestationLen_d', 'X26.4_GR_MidRangeLat_dd'),
        parallel = TRUE, plot = TRUE)
```

```
## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'

## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'
```



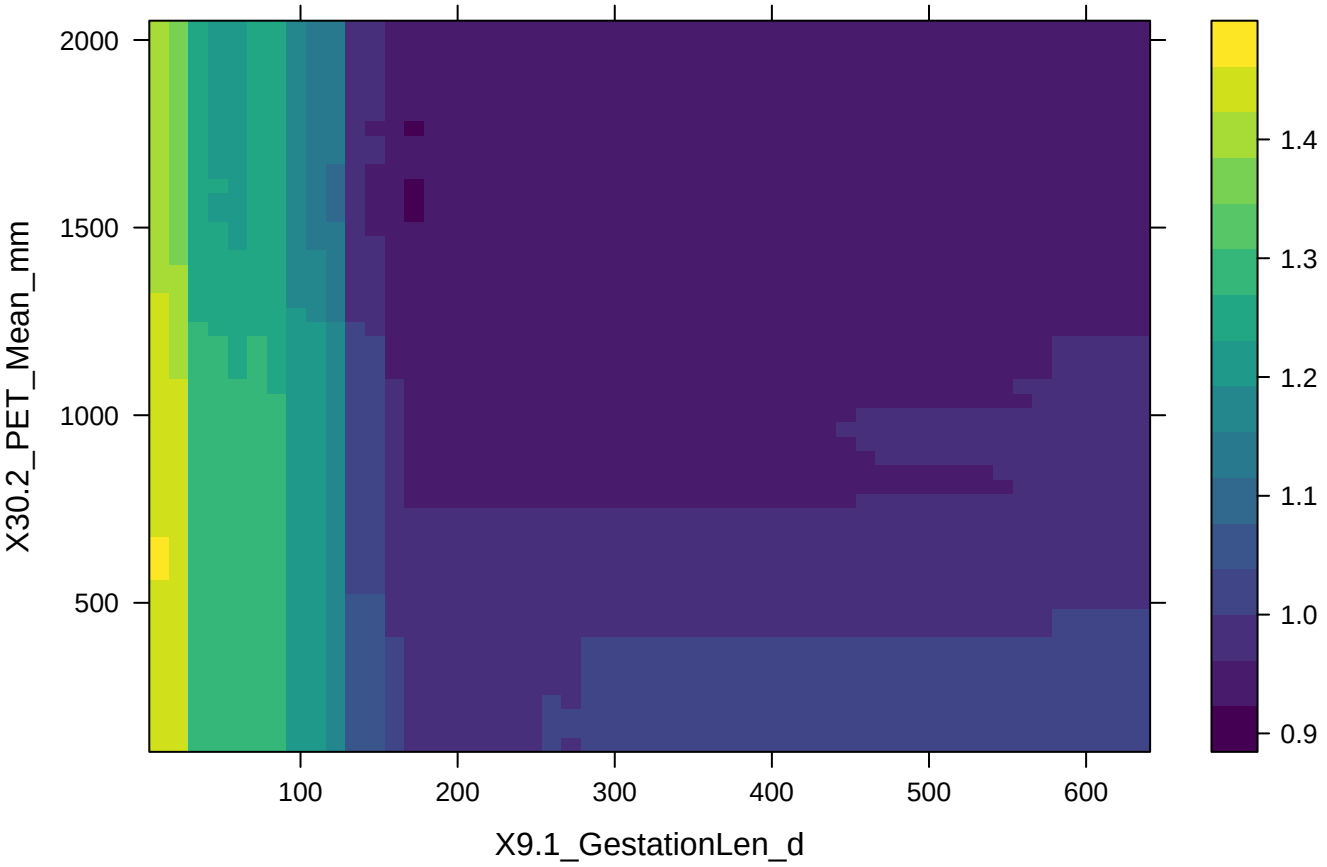

```
partial(m2_gp,
        pred.var = c('X9.1_GestationLen_d', 'X30.2_PET_Mean_mm'),
        parallel = TRUE, plot = TRUE)
```

```
## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'

## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'
```




```
partial(m3_rf,
        pred.var = c('X9.1_GestationLen_d', 'X30.2_PET_Mean_mm'),
        parallel = TRUE, plot = TRUE)
```

```
## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'

## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'
```

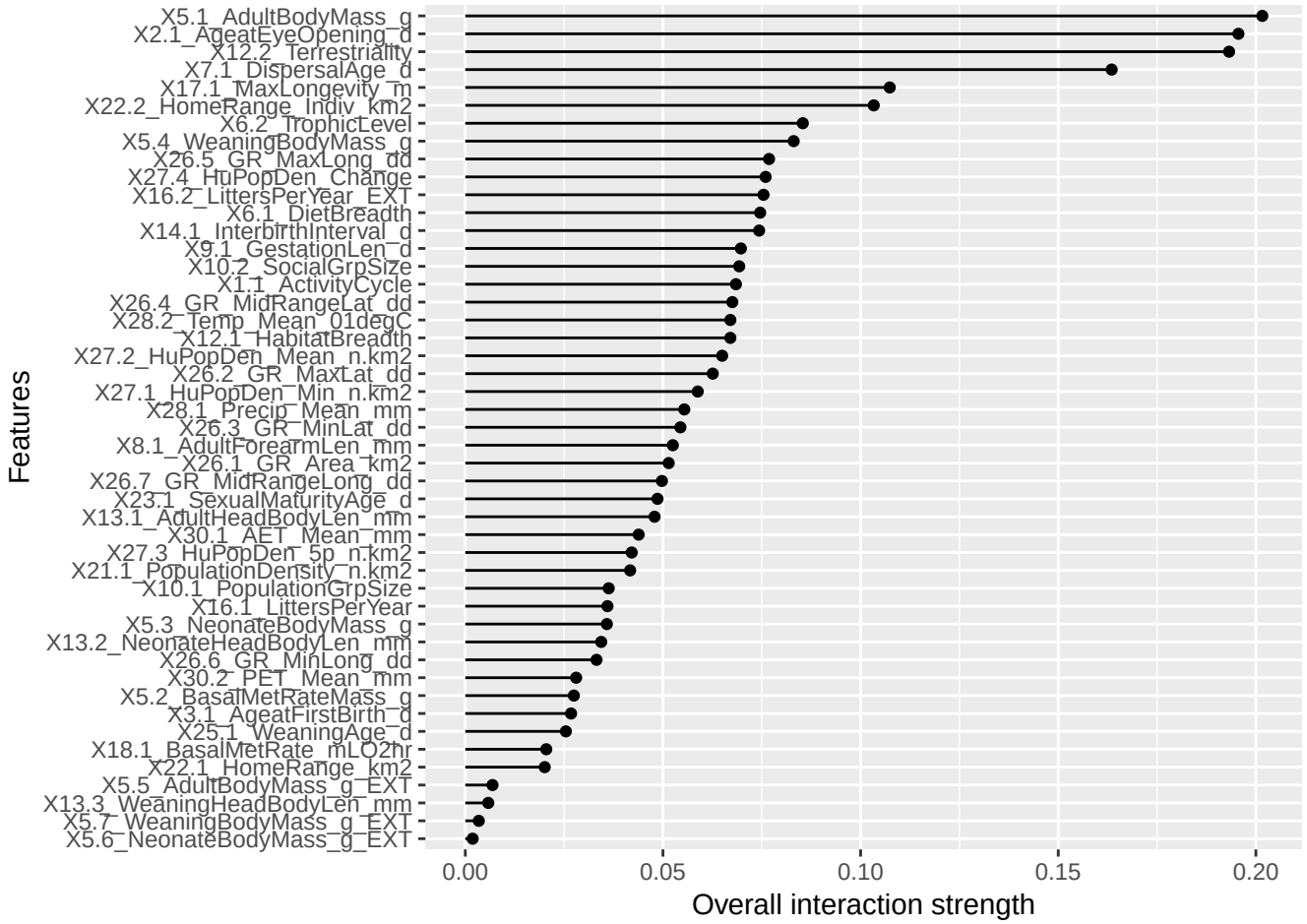


Test for interactions

```
predictor_gp = Predictor$new(m2_gp, data = dplyr::select(p_impute, -y), y = p_impute$y)
predictor_rf = Predictor$new(m3_rf, data = dplyr::select(p_impute, -y), y = p_impute$y)


interact_gp = Interaction$new(predictor_gp)
interact_gp$results %>% arrange(desc(.interaction)) %>% head
```

```
##                     .feature .interaction
## 1      X5.1_AdultBodyMass_g    0.2016154
## 2    X2.1_AgeatEyeOpening_d    0.1955797
## 3      X12.2_Terrestriality    0.1932190
## 4       X7.1_DispersalAge_d    0.1635105
## 5      X17.1_MaxLongevity_m    0.1073744
## 6 X22.2_HomeRange_Indiv_km2    0.1033276
```

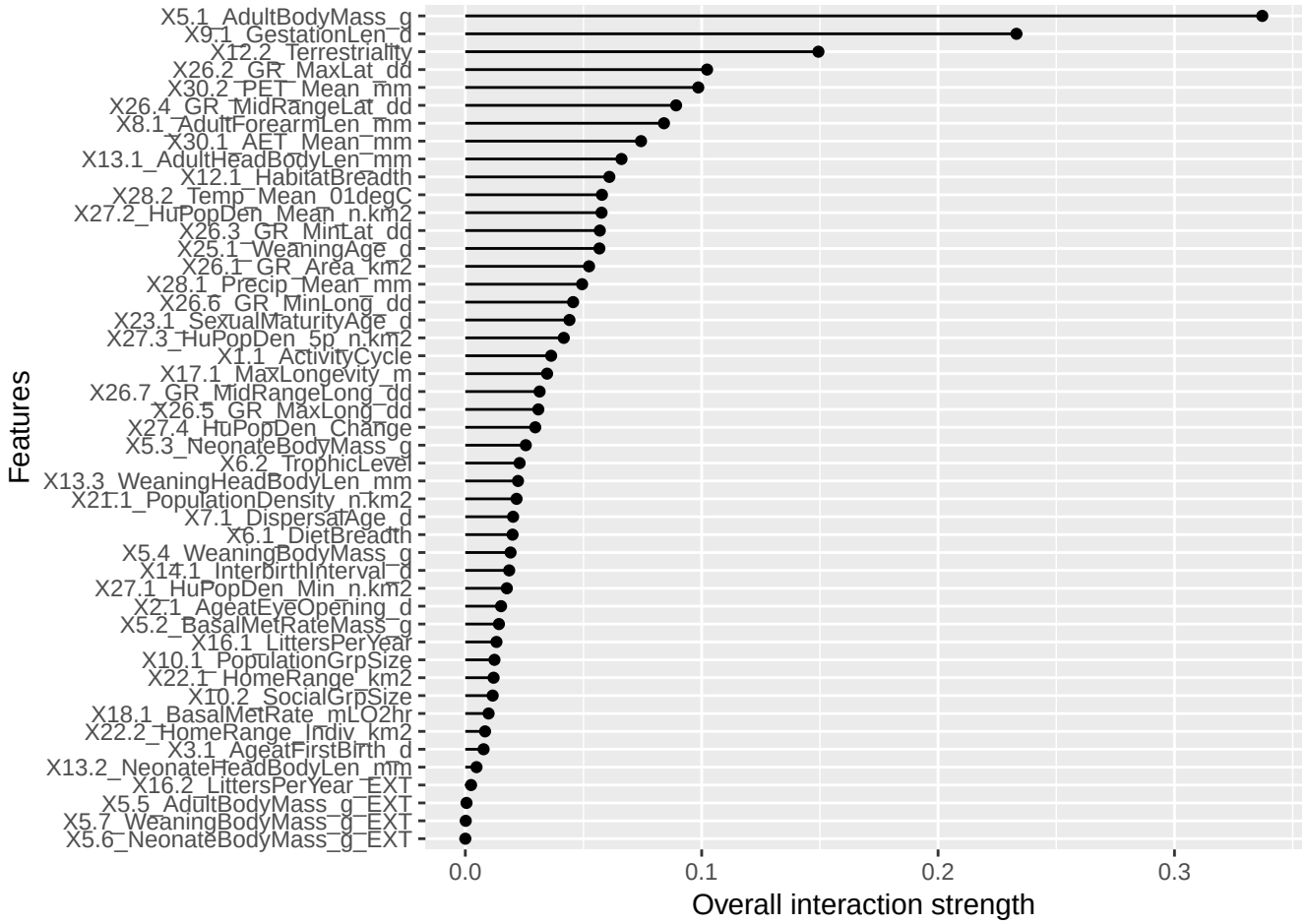
```
plot(interact_gp)
```




```
interact_rf = Interaction$new(predictor_rf)
interact_rf$results %>% arrange(desc(.interaction)) %>% head
```

```
##                  .feature .interaction
## 1    X5.1_AdultBodyMass_g    0.3371445
## 2     X9.1_GestationLen_d    0.2331598
## 3    X12.2_Terrestriality    0.1493818
## 4      X26.2_GR_MaxLat_dd    0.1022850
## 5       X30.2_PET_Mean_mm    0.0985487
## 6 X26.4_GR_MidRangeLat_dd    0.0891687
```

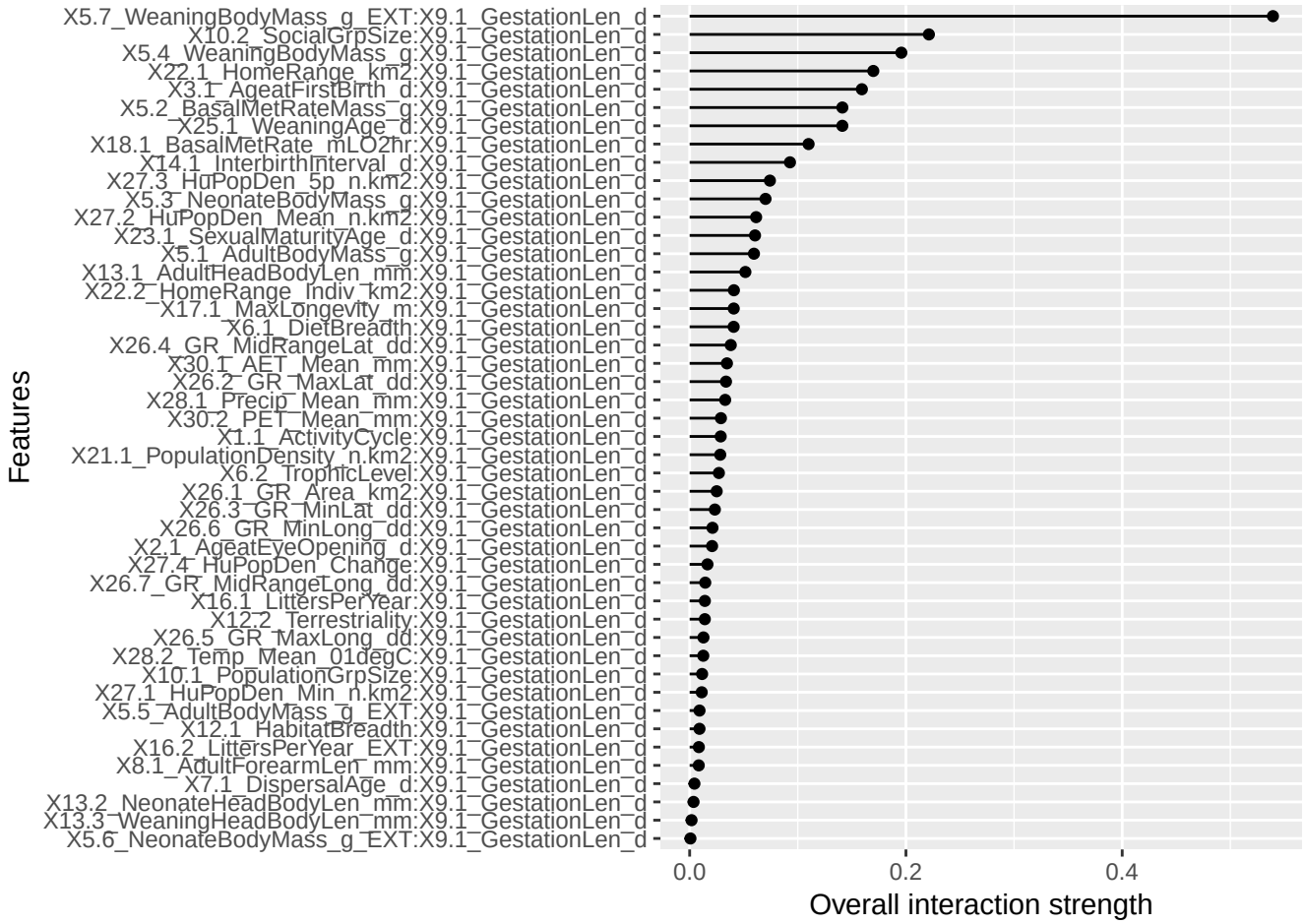
```
plot(interact_rf)
```




```
interact_ges_gp = Interaction$new(predictor_gp, feature = "X9.1_GestationLen_d")
interact_ges_gp$results %>% arrange(desc(.interaction)) %>% head
```

```
##                                        .feature .interaction
## 1 X5.7_WeaningBodyMass_g_EXT:X9.1_GestationLen_d    0.5393717
## 2        X10.2_SocialGrpSize:X9.1_GestationLen_d    0.2212288
## 3     X5.4_WeaningBodyMass_g:X9.1_GestationLen_d    0.1957718
## 4        X22.1_HomeRange_km2:X9.1_GestationLen_d    0.1698334
## 5     X3.1_AgeatFirstBirth_d:X9.1_GestationLen_d    0.1592361
## 6    X5.2_BasalMetRateMass_g:X9.1_GestationLen_d    0.1412126
```

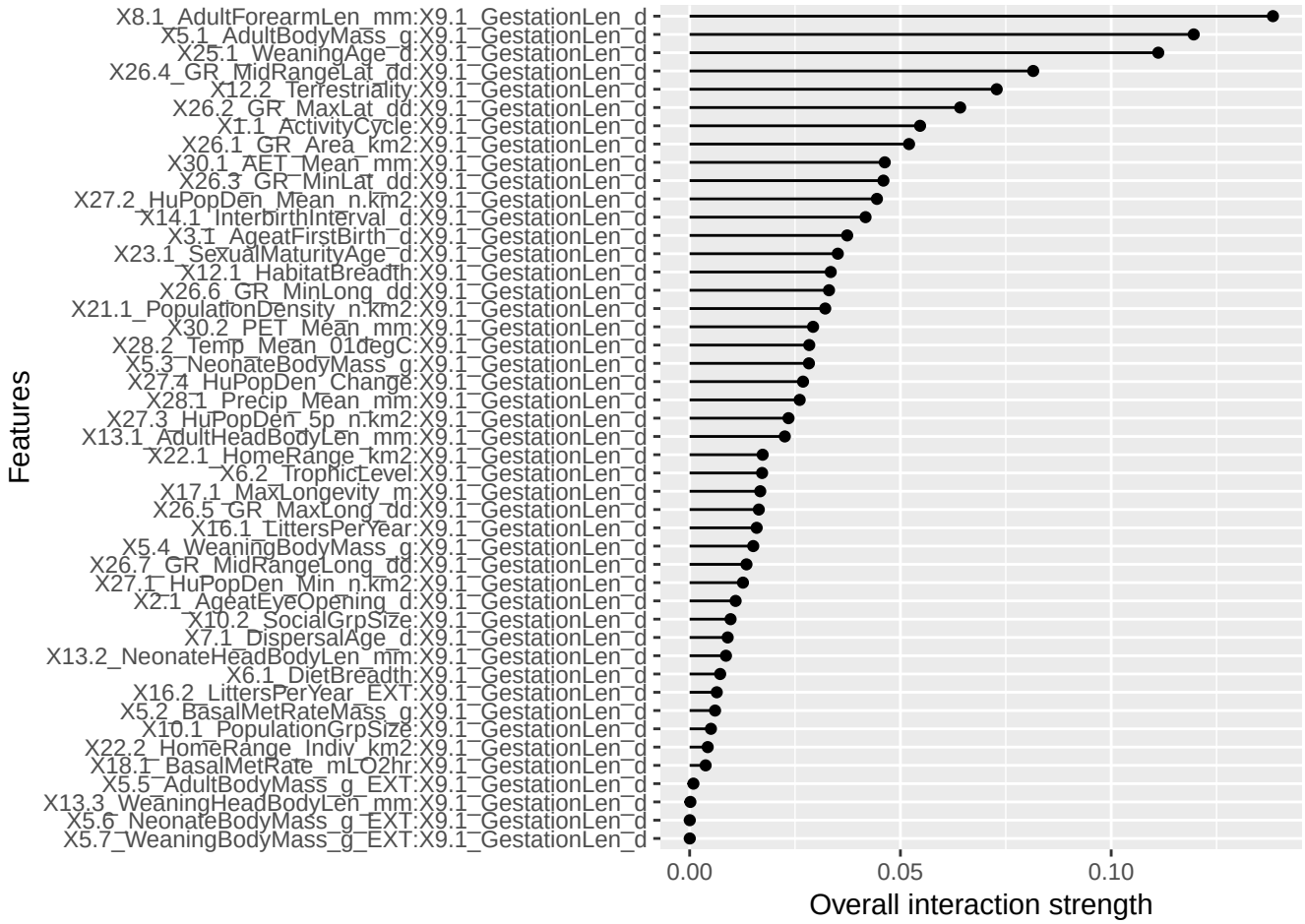
```
plot(interact_ges_gp)
```




```
interact_ges_rf = Interaction$new(predictor_rf, feature = "X9.1_GestationLen_d")
interact_ges_rf$results %>% arrange(desc(.interaction)) %>% head
```

```
##                                     .feature .interaction
## 1 X8.1_AdultForearmLen_mm:X9.1_GestationLen_d   0.13836986
## 2    X5.1_AdultBodyMass_g:X9.1_GestationLen_d   0.11957721
## 3      X25.1_WeaningAge_d:X9.1_GestationLen_d   0.11116702
## 4 X26.4_GR_MidRangeLat_dd:X9.1_GestationLen_d   0.08149829
## 5    X12.2_Terrestriality:X9.1_GestationLen_d   0.07283942
## 6      X26.2_GR_MaxLat_dd:X9.1_GestationLen_d   0.06417600
```

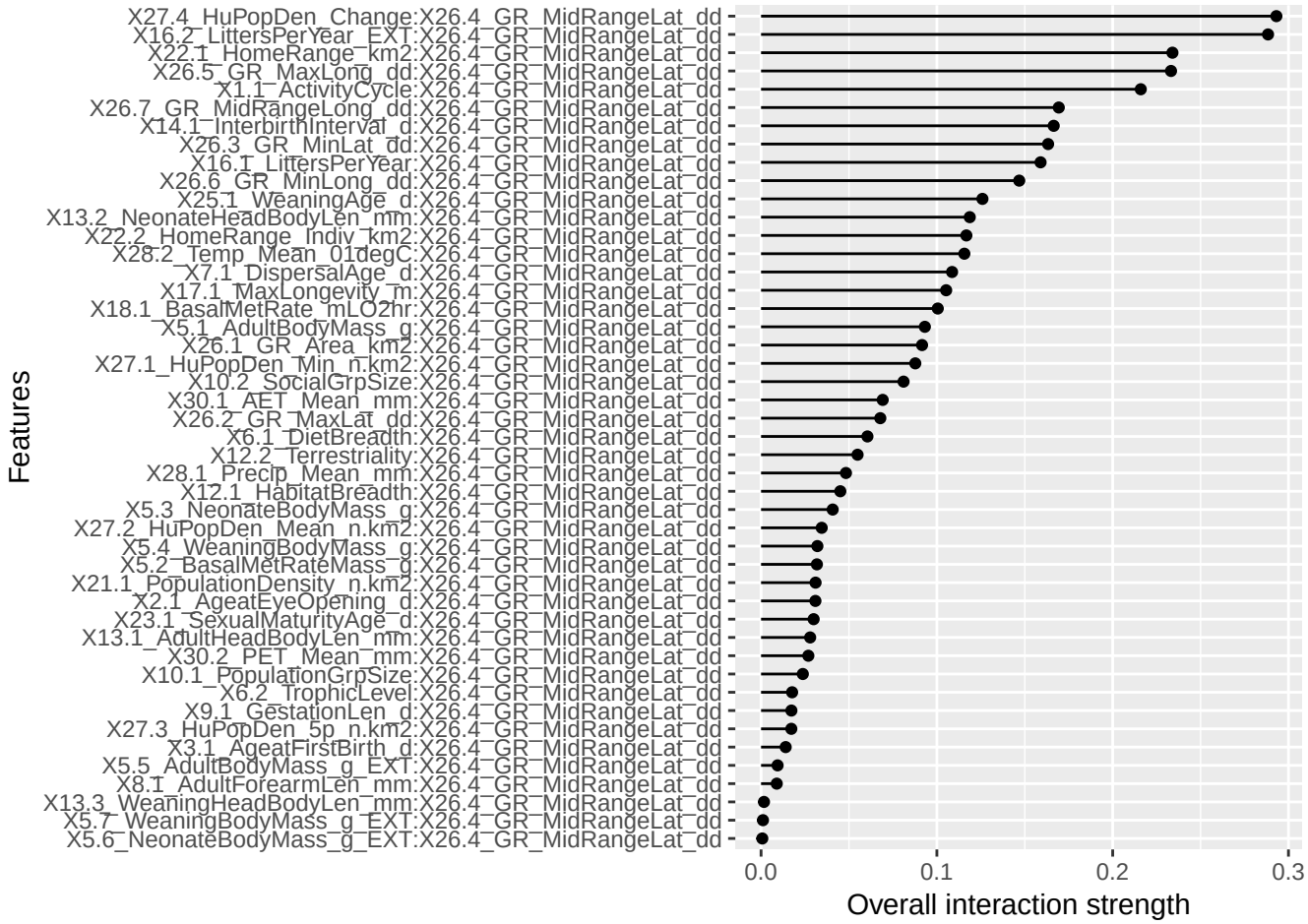
```
plot(interact_ges_rf)
```




```
interact_lat_gp = Interaction$new(predictor_gp, feature = "X26.4_GR_MidRangeLat_dd")
interact_lat_gp$results %>% arrange(desc(.interaction)) %>% head
```

```
##                                          .feature .interaction
## 1    X27.4_HuPopDen_Change:X26.4_GR_MidRangeLat_dd    0.2931253
## 2 X16.2_LittersPerYear_EXT:X26.4_GR_MidRangeLat_dd    0.2883728
## 3      X22.1_HomeRange_km2:X26.4_GR_MidRangeLat_dd    0.2339927
## 4      X26.5_GR_MaxLong_dd:X26.4_GR_MidRangeLat_dd    0.2331797
## 5       X1.1_ActivityCycle:X26.4_GR_MidRangeLat_dd    0.2159893
## 6 X26.7_GR_MidRangeLong_dd:X26.4_GR_MidRangeLat_dd    0.1693449
```

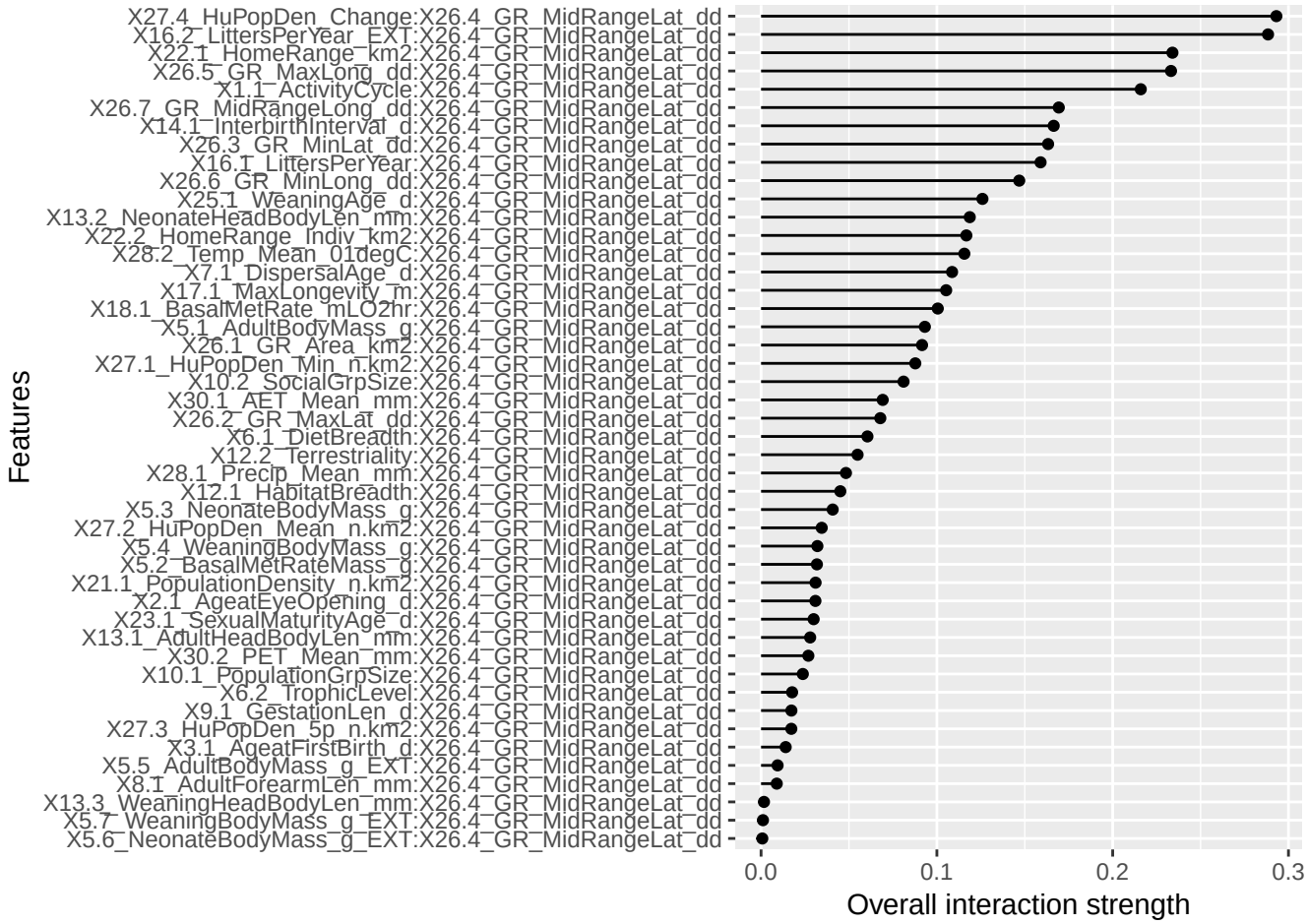
```
plot(interact_lat_gp)
```




```
interact_lat_rf = Interaction$new(predictor_rf, feature = "X26.4_GR_MidRangeLat_dd")
interact_lat_rf$results %>% arrange(desc(.interaction)) %>% head
```

```
##                                          .feature .interaction
## 1   X8.1_AdultForearmLen_mm:X26.4_GR_MidRangeLat_dd    0.1465875
## 2      X5.1_AdultBodyMass_g:X26.4_GR_MidRangeLat_dd    0.1254077
## 3      X28.1_Precip_Mean_mm:X26.4_GR_MidRangeLat_dd    0.1199153
## 4 X23.1_SexualMaturityAge_d:X26.4_GR_MidRangeLat_dd    0.1097579
## 5      X17.1_MaxLongevity_m:X26.4_GR_MidRangeLat_dd    0.1081483
## 6       X9.1_GestationLen_d:X26.4_GR_MidRangeLat_dd    0.0948204
```

```
plot(interact_lat_gp)
```

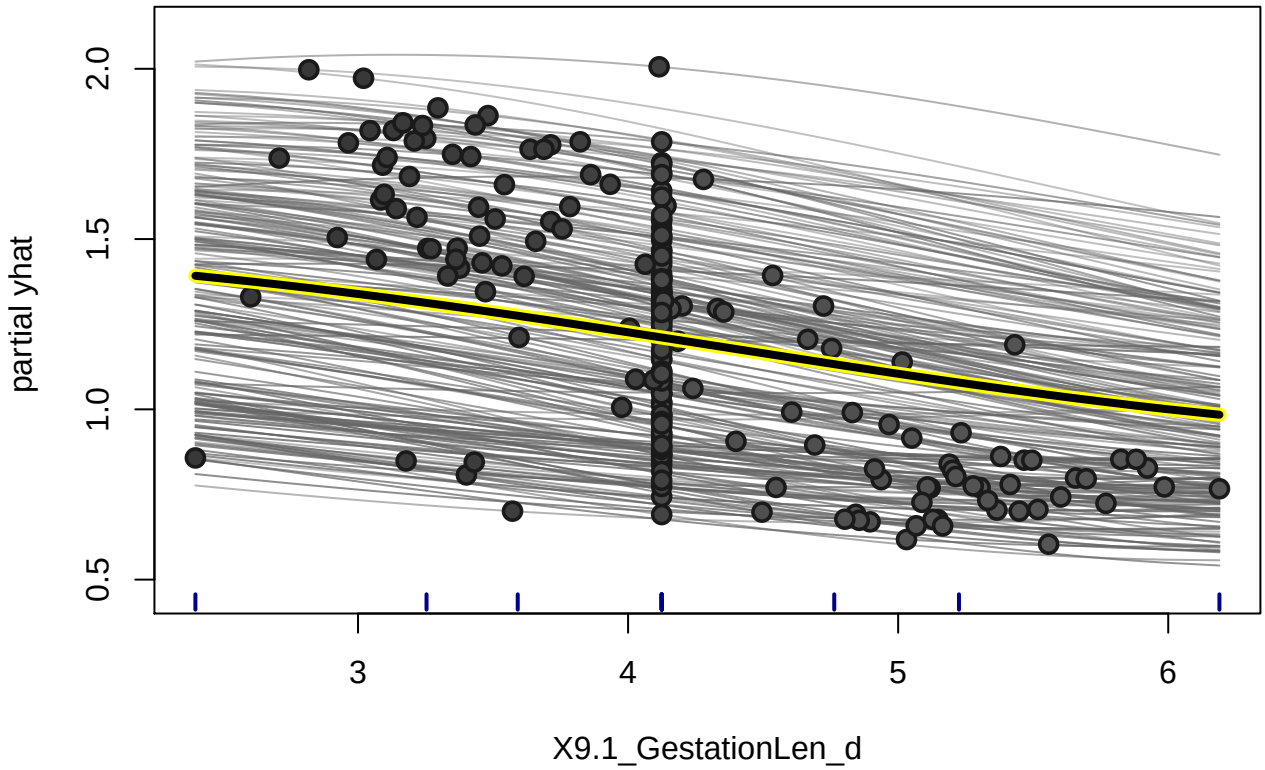


ICE plots

```
m2_gp_ice <- ice(m2_gp, p_impute, p_impute$y, 'X9.1_GestationLen_d', frac_to_build = 0.1)
```

```
## ..................................................................................................................................
```

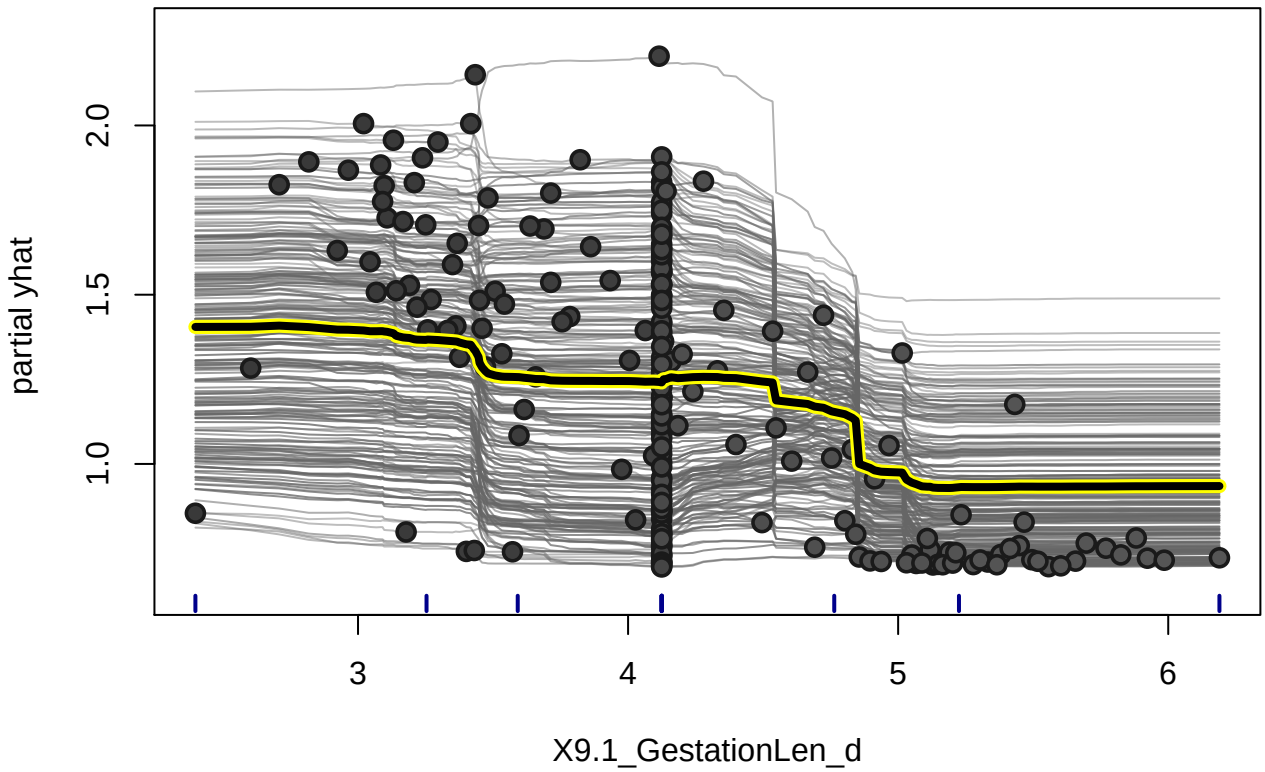
```
plot(m2_gp_ice)
```




```
m3_rf_ice <- ice(m3_rf, p_impute, p_impute$y, 'X9.1_GestationLen_d', frac_to_build = 0.1)
```

```
## ..................................................................................................
```

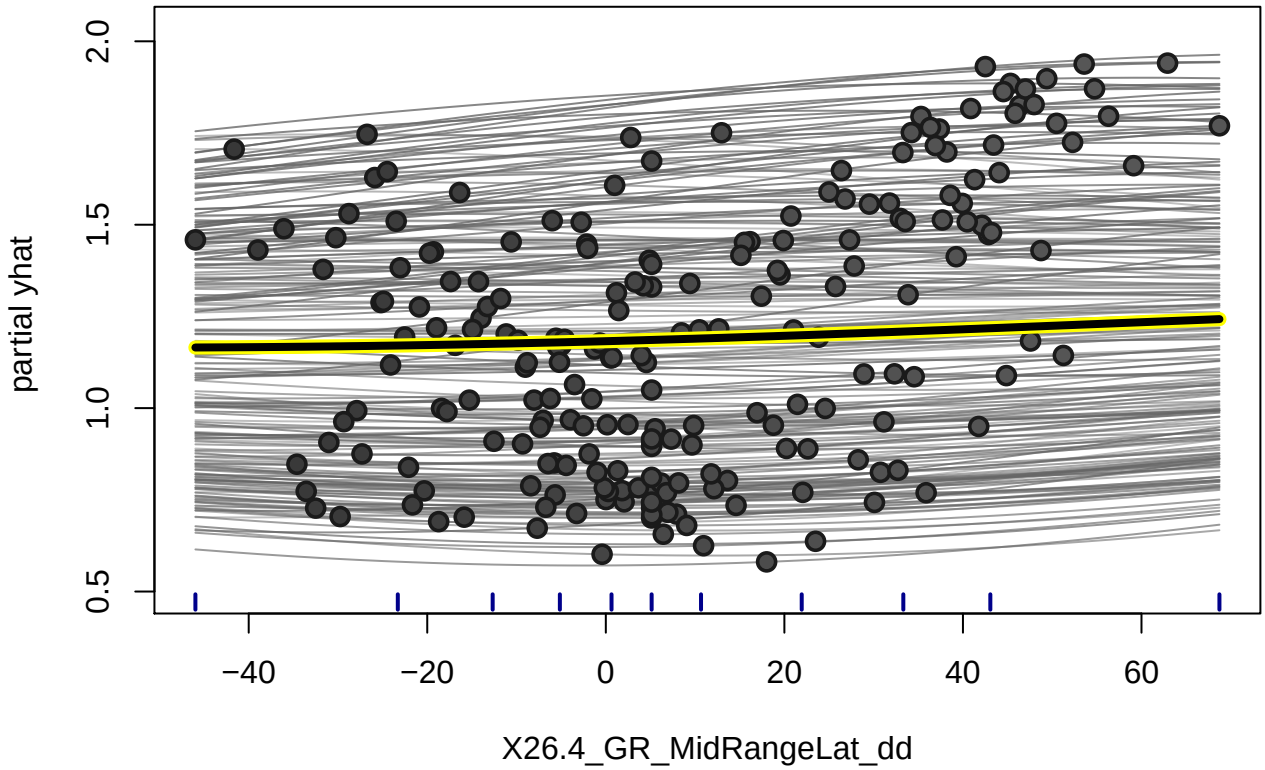
```
plot(m3_rf_ice)
```




```
m2_gp_ice_lat <- ice(m2_gp, p_impute, p_impute$y, 'X26.4_GR_MidRangeLat_dd', frac_to_build = 0.1)
```

```
## ..................................................................................................
```

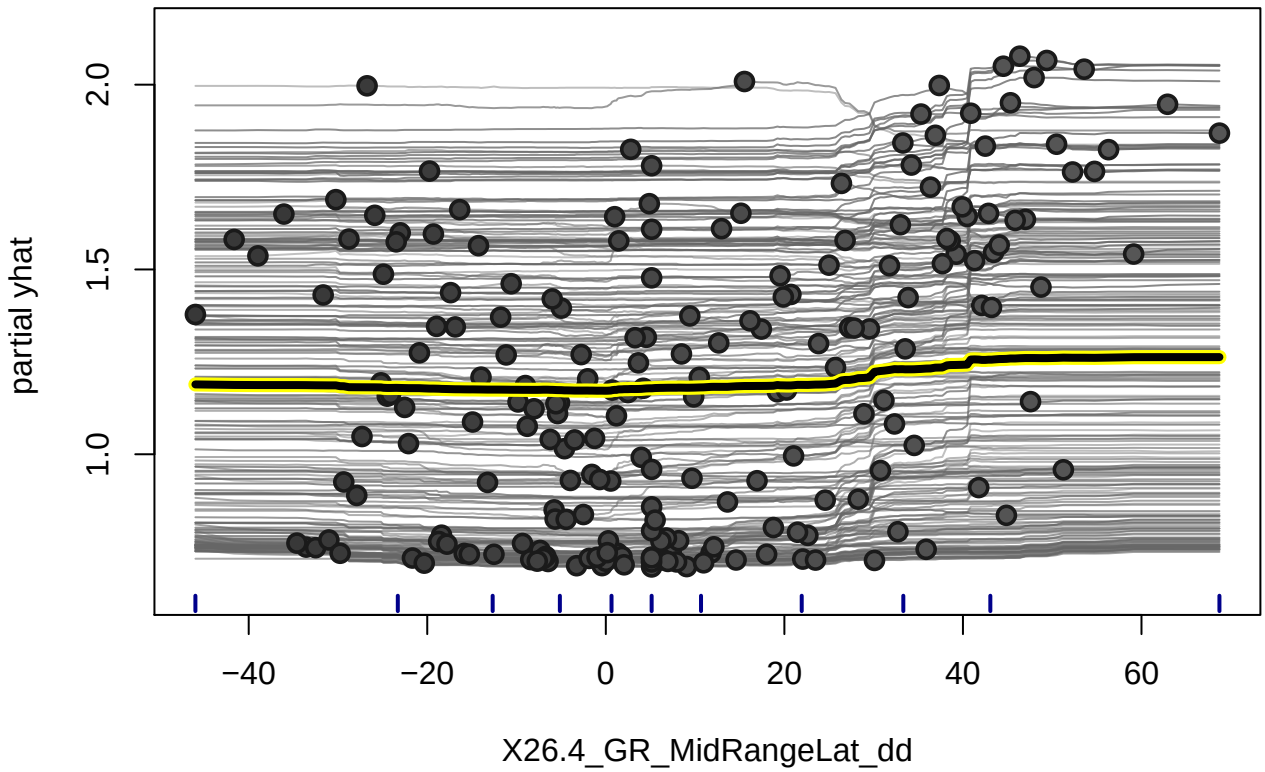
```
plot(m2_gp_ice_lat)
```




```
m3_rf_ice_lat <- ice(m3_rf, p_impute, p_impute$y, 'X26.4_GR_MidRangeLat_dd', frac_to_build = 0.1)
```

```
## ..................................................................................................
```

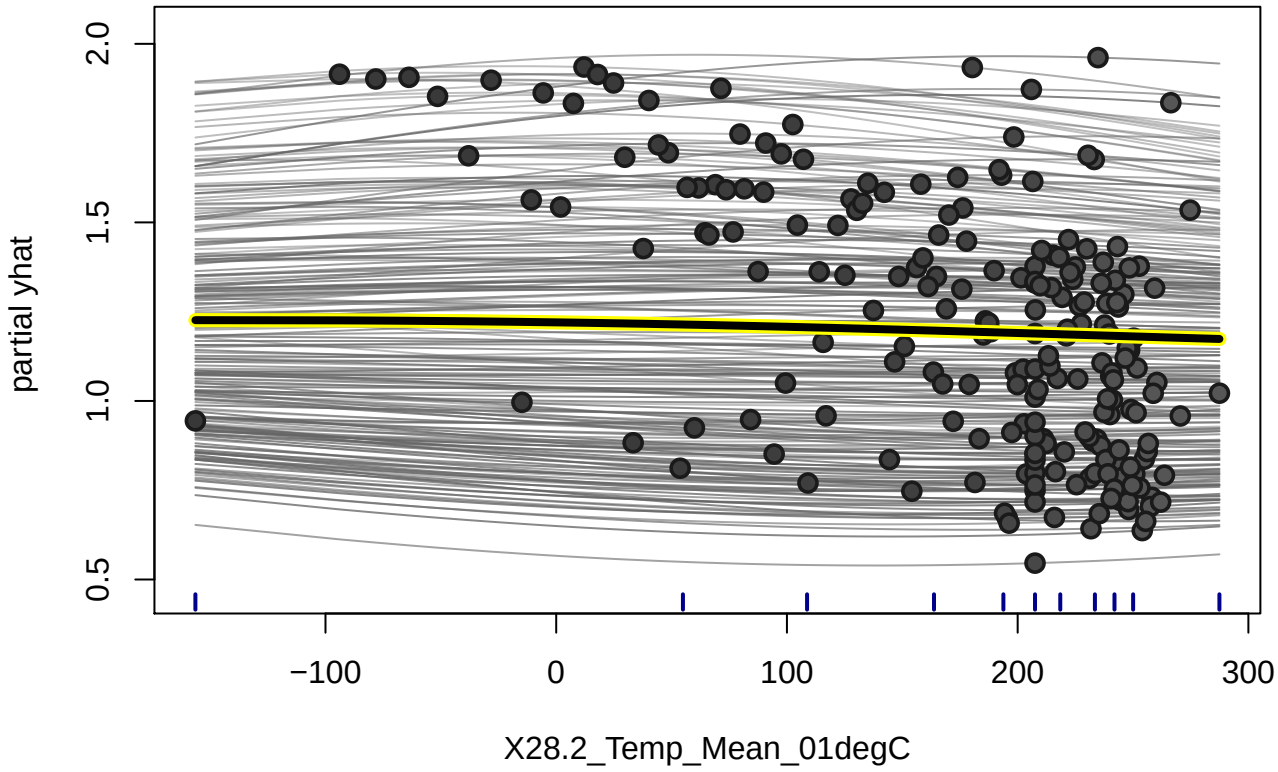
```
plot(m3_rf_ice_lat)
```




```
m2_gp_ice_temp <- ice(m2_gp, p_impute, p_impute$y, 'X28.2_Temp_Mean_01degC', frac_to_build = 0.1)
```

```
## ..................................................................................................
```

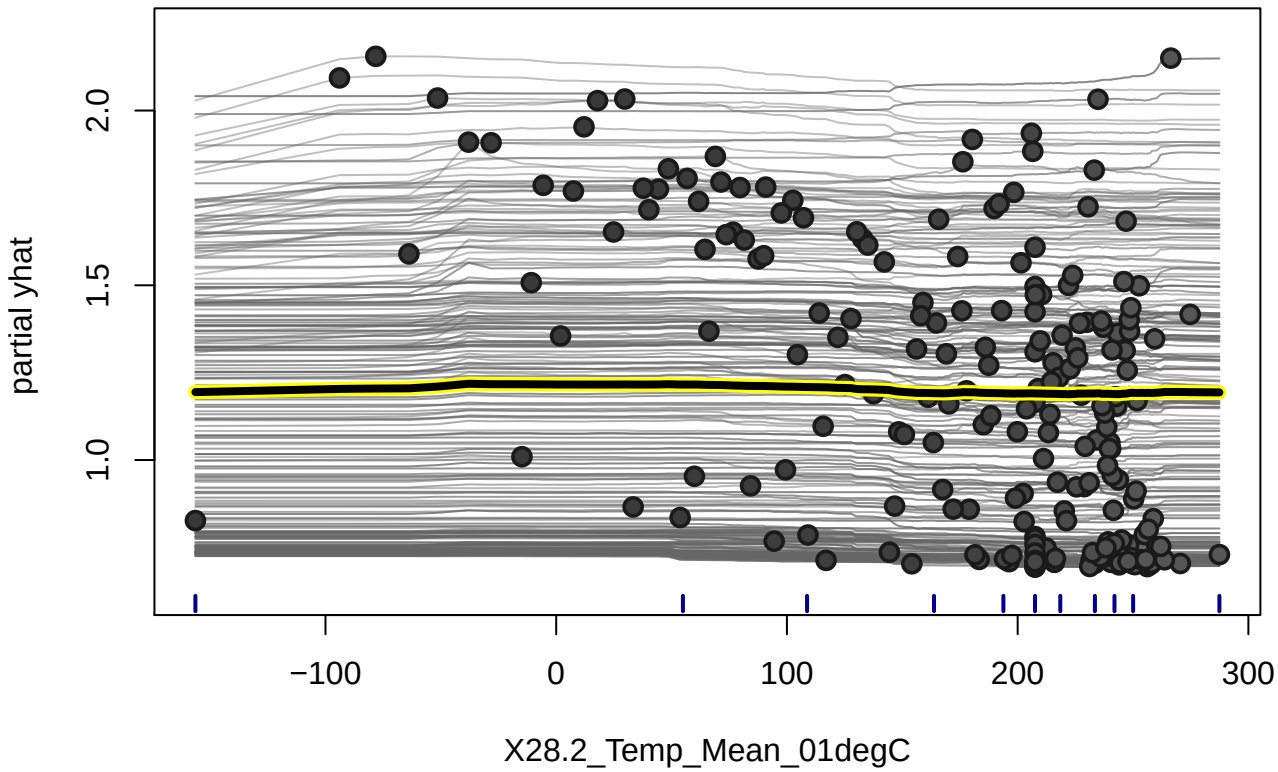
```
plot(m2_gp_ice_temp)
```




```
m3_rf_ice_temp <- ice(m3_rf, p_impute, p_impute$y, 'X28.2_Temp_Mean_01degC', frac_to_build = 0.1)
```

```
## ..........................................................................................................
```

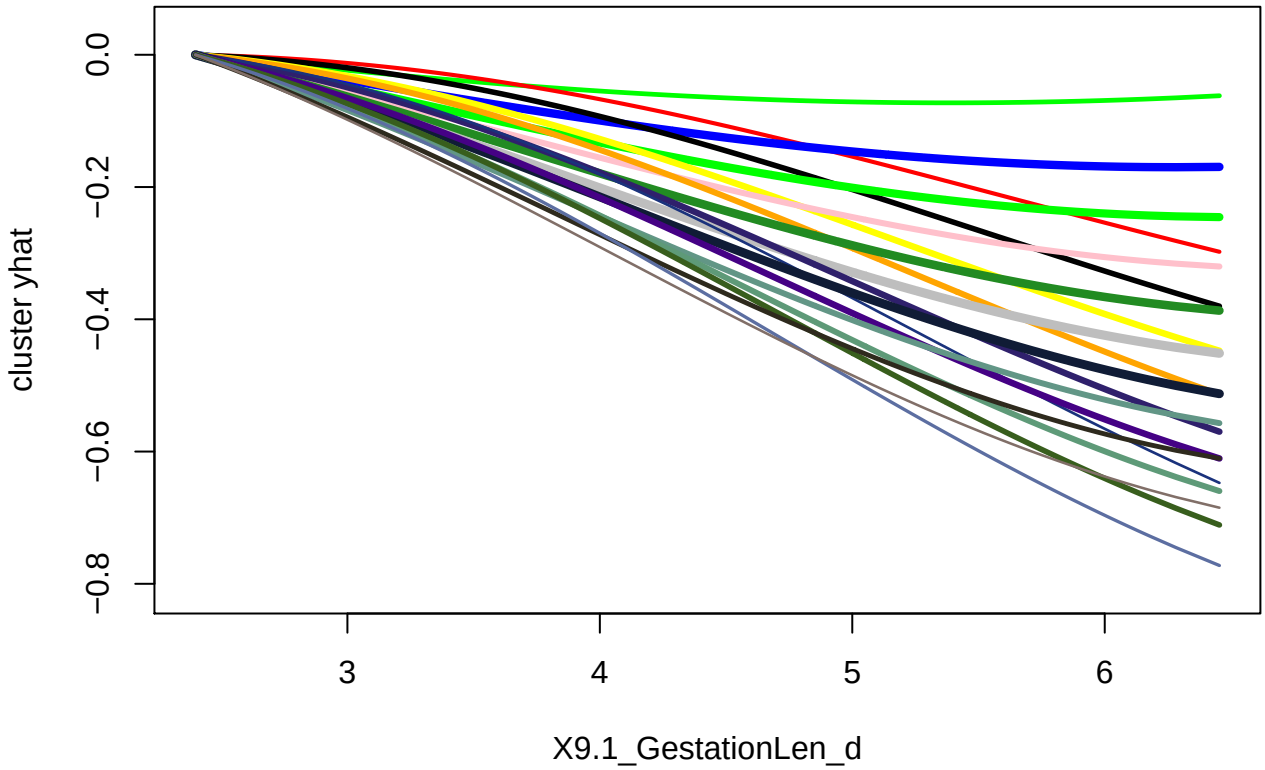
```
plot(m3_rf_ice_temp)
```



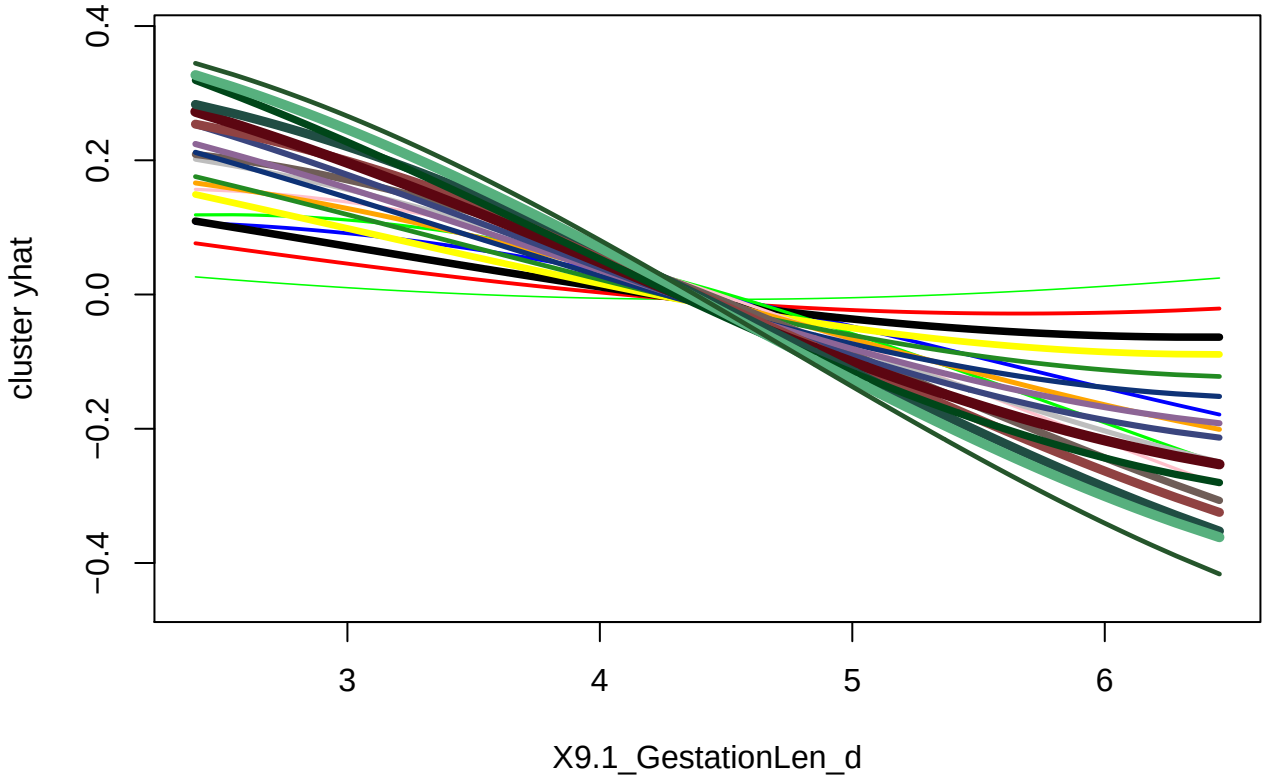

```
m2_gp_ice_c <- ice(m2_gp, p_impute, p_impute$y, 'X9.1_GestationLen_d')
```

```
## ..........................................................................................................
```

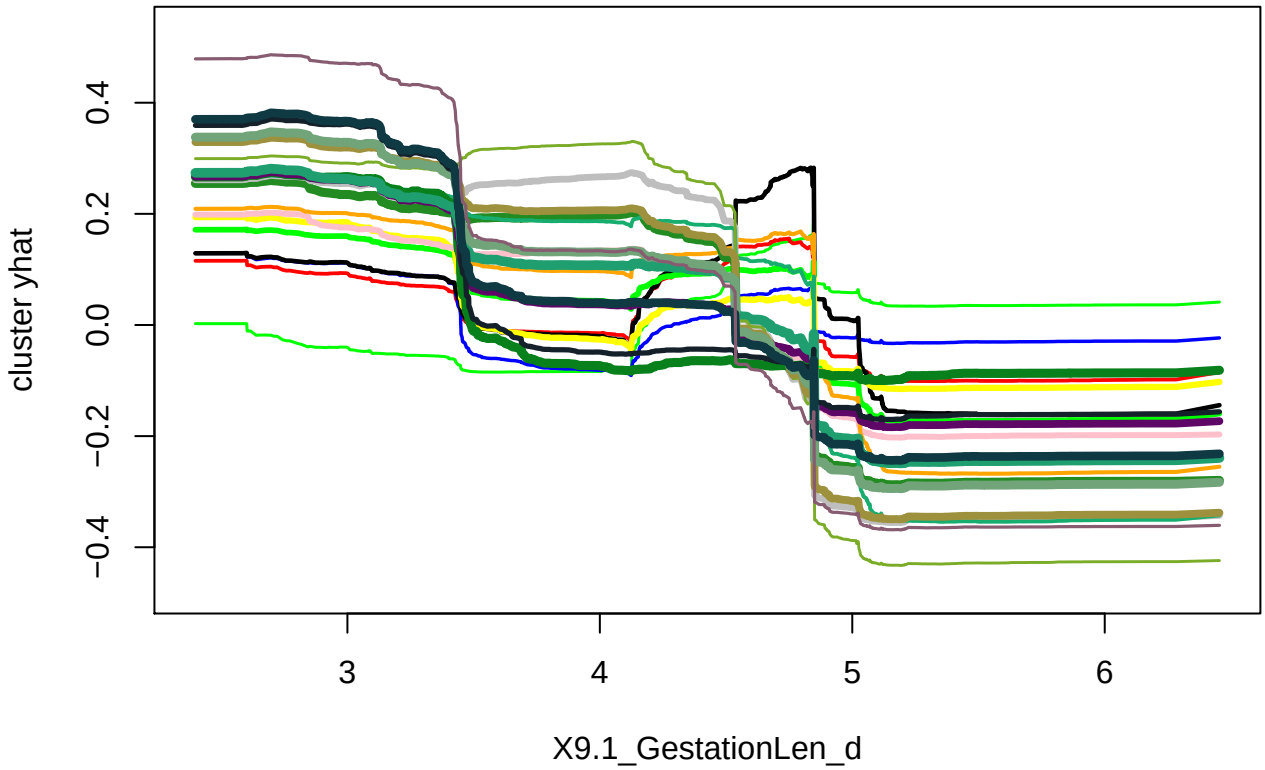
```
clusterICE(m2_gp_ice_c, nClusters = 20, centered = TRUE)
```




```
clusterICE(m2_gp_ice_c, nClusters = 20, centered = FALSE)
```



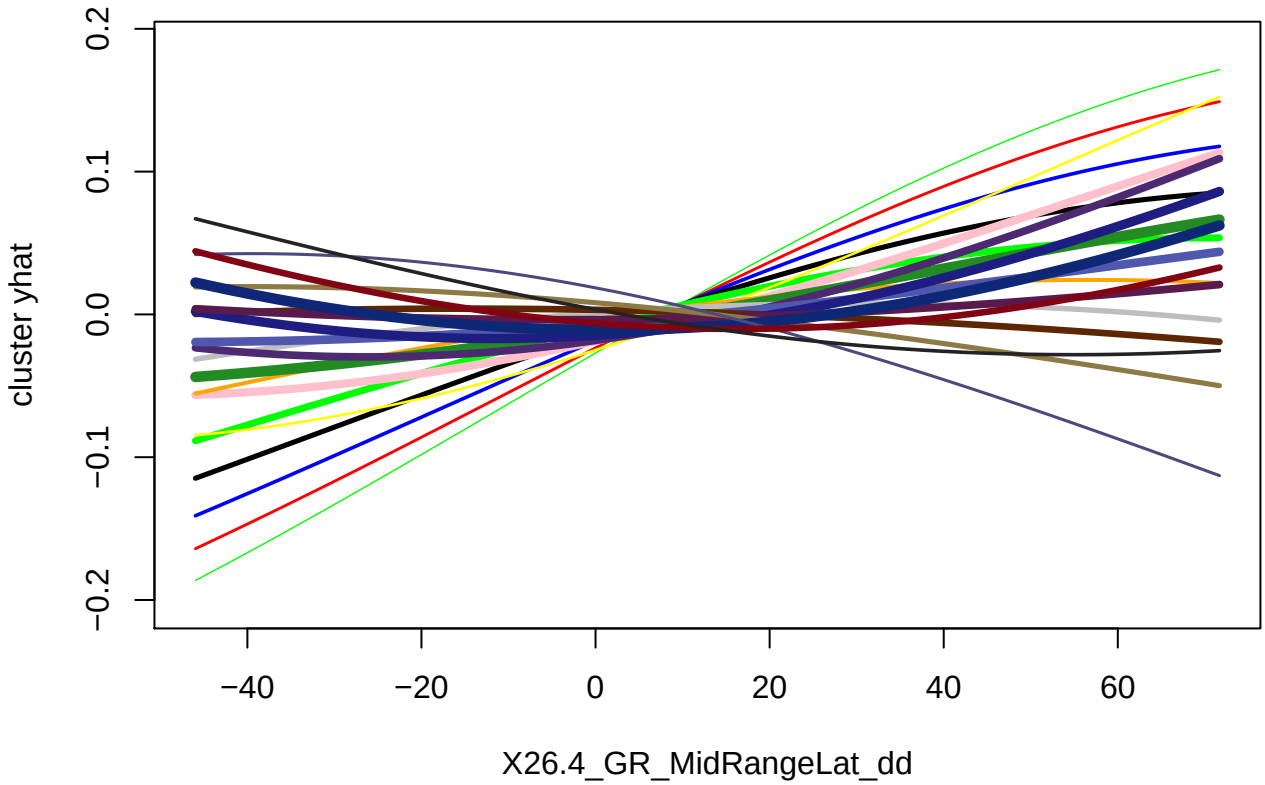

```
m3_rf_ice_c <- ice(m3_rf, p_impute, p_impute$y, 'X9.1_GestationLen_d')

## ..........................................................................................................
clusterICE(m3_rf_ice_c, nClusters = 20, centered = FALSE)
```




```
m2_gp_ice_lat_c <- ice(m2_gp, p_impute, p_impute$y, 'X26.4_GR_MidRangeLat_dd')
```

```
## ..............................................................................................................
```

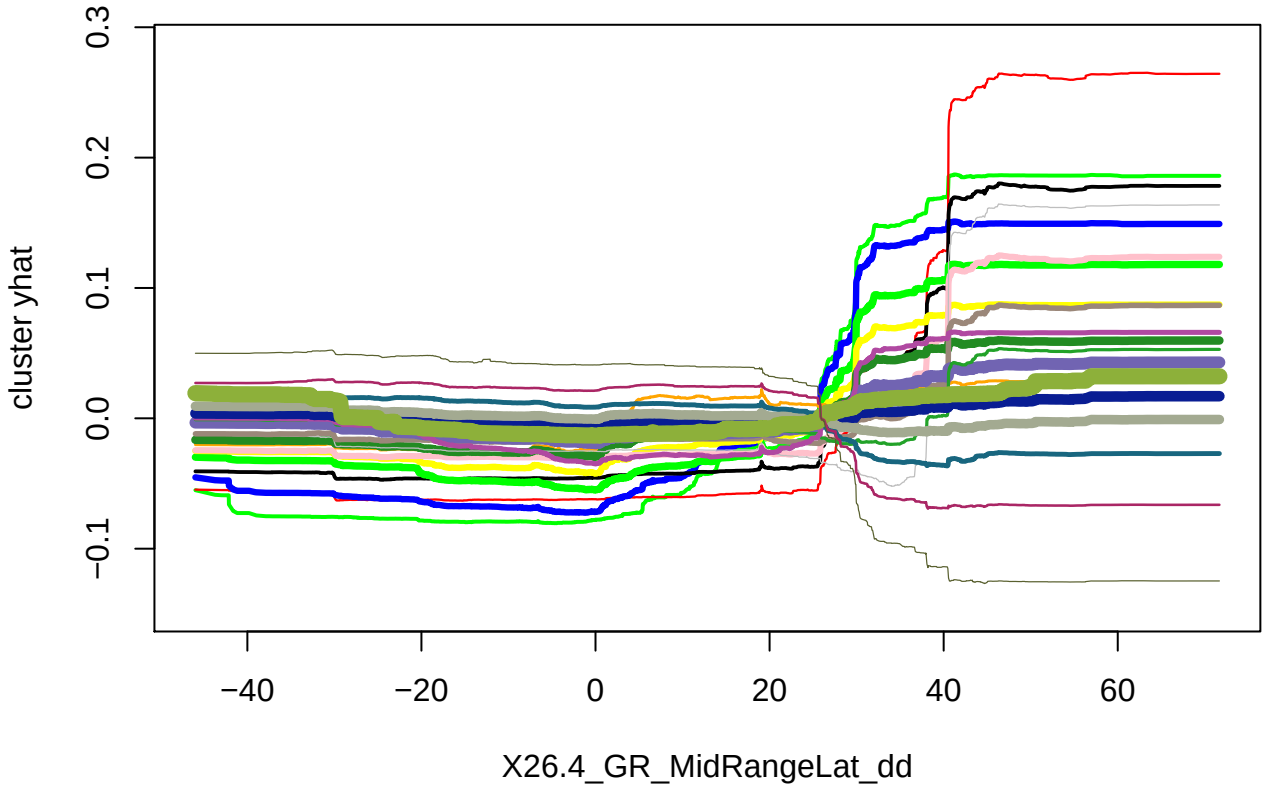
```
clusterICE(m2_gp_ice_lat_c, nClusters = 20, centered = FALSE)
```




```
m3_rf_ice_lat_c <- ice(m3_rf, p_impute, p_impute$y, 'X26.4_GR_MidRangeLat_dd')
```

```
## ..............................................................................................................
```

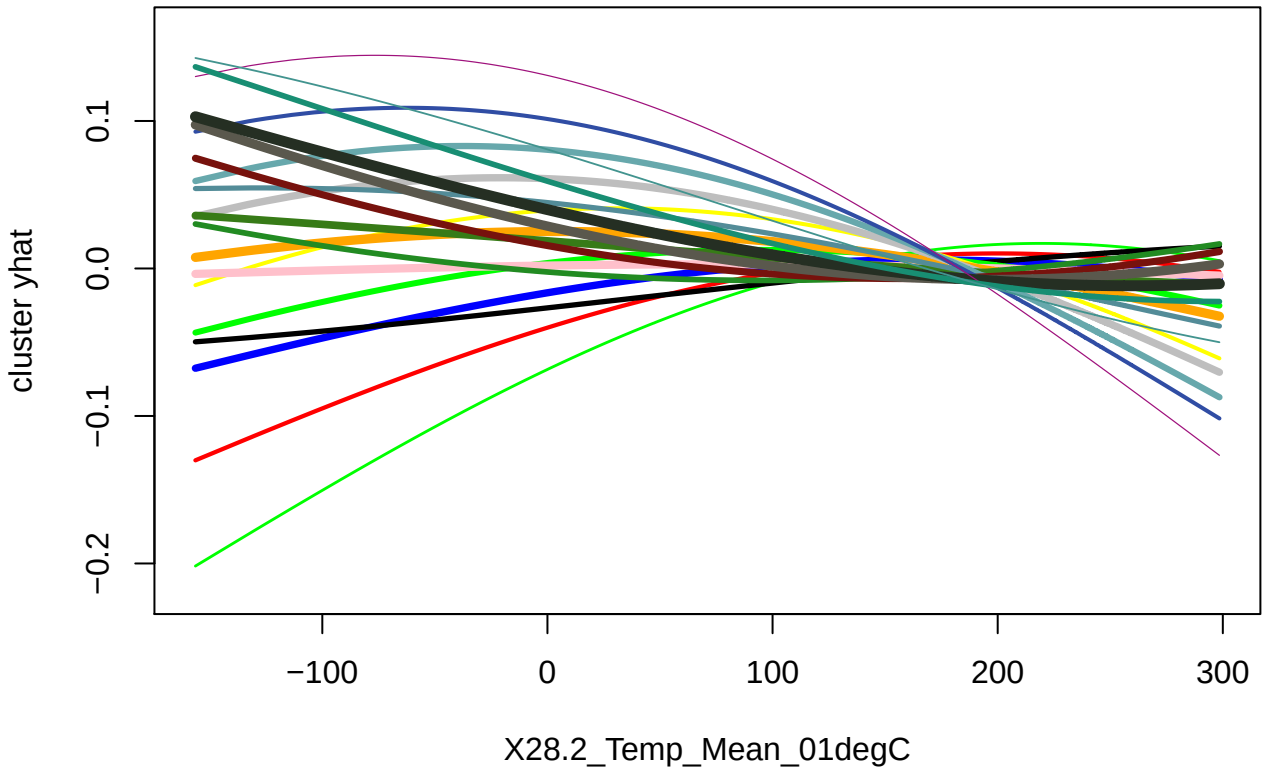
```
clusterICE(m3_rf_ice_lat_c, nClusters = 20, centered = FALSE)
```




```
m2_gp_ice_temp_c <- ice(m2_gp, p_impute, p_impute$y, 'X28.2_Temp_Mean_01degC')
```

```
## ..............................................................................................................
```

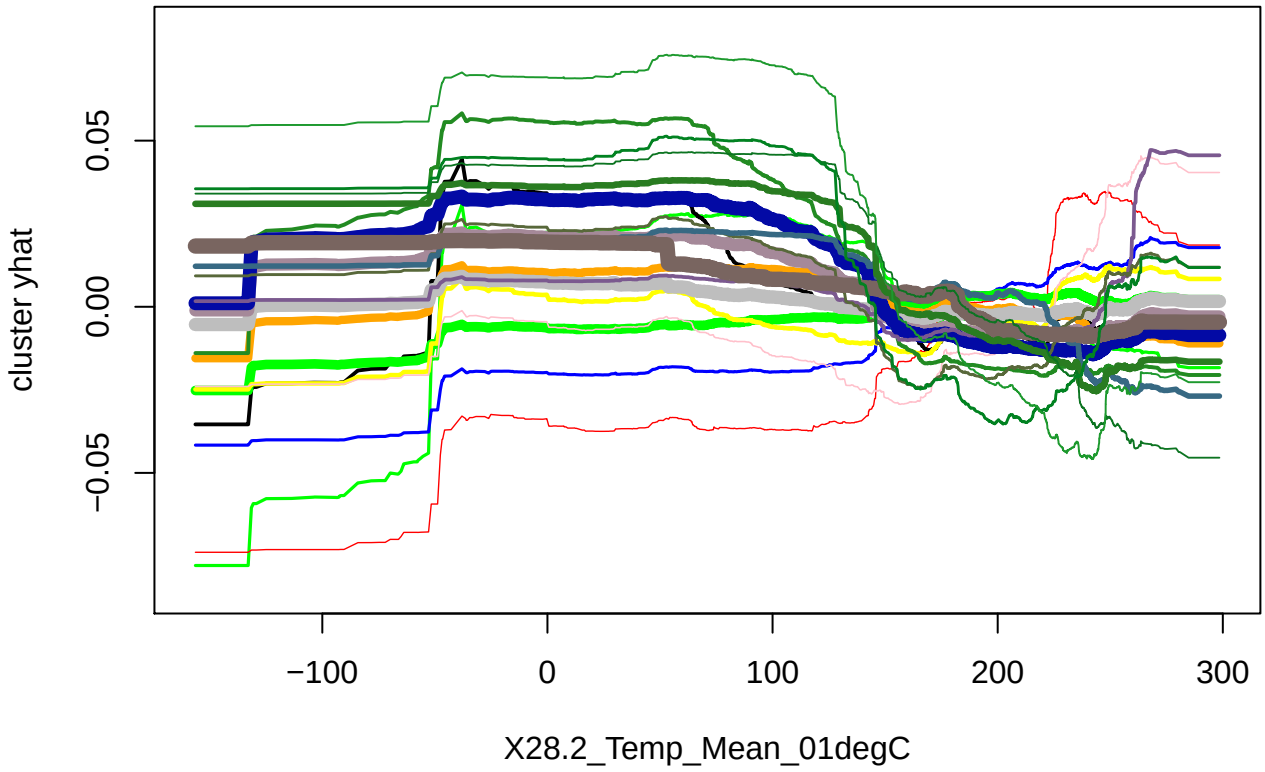
```
clusterICE(m2_gp_ice_temp_c, nClusters = 20, centered = FALSE)
```




```
m3_rf_ice_temp_c <- ice(m3_rf, p_impute, p_impute$y, 'X28.2_Temp_Mean_01degC')
```

```
## ..............................................................................................................
```

```
clusterICE(m3_rf_ice_temp_c, nClusters = 20, centered = FALSE)
```



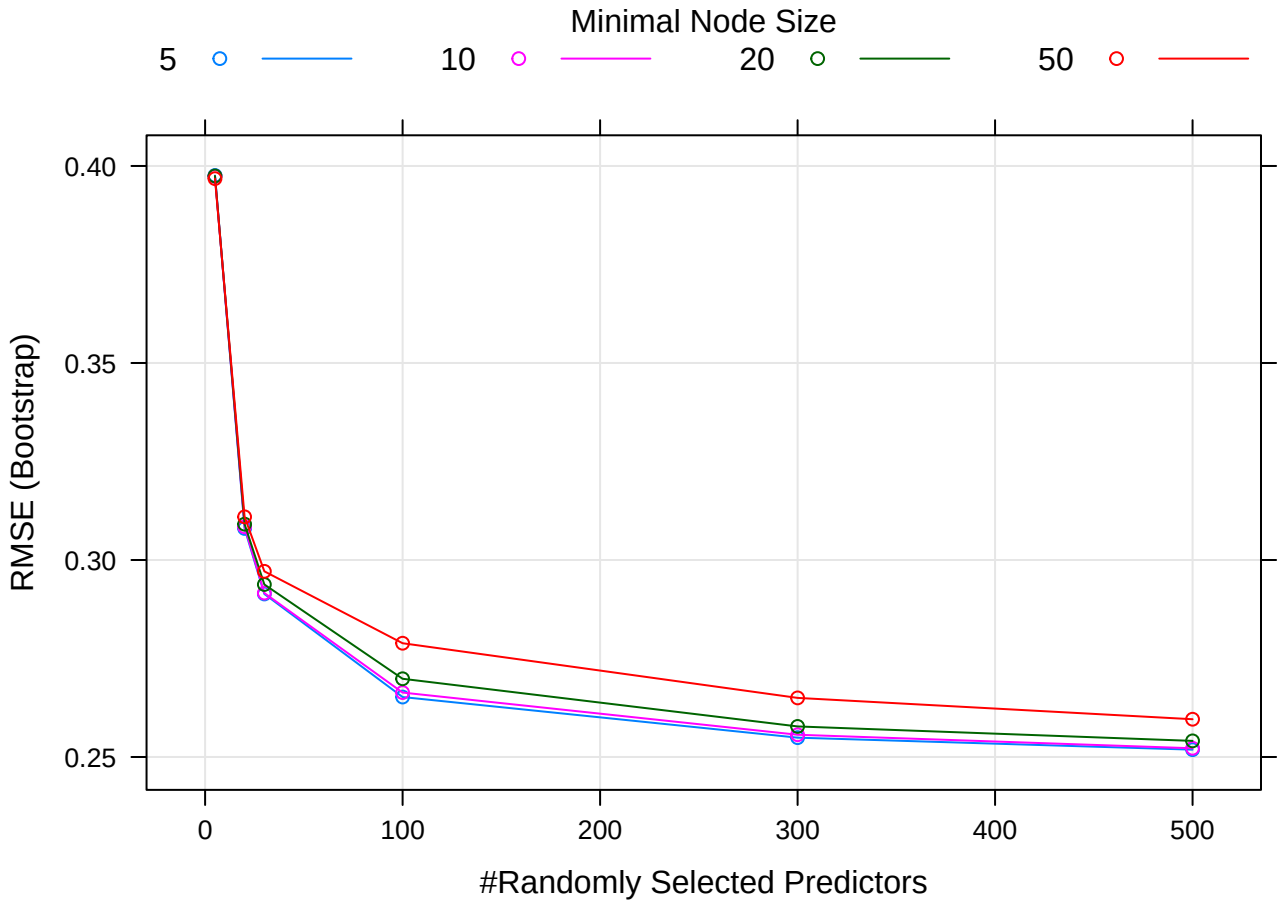
Examine correlation structure

- examine correlation structure (variable level)
  - random effects
  - mean zero
  - unseen values
  - control Vs use in prediction
  - shared power
  - feature engineering (eg t-1 value)
  - stacked generalisation
  - priors
  - random slopes are regularised interactions. dealt with fairly natively by RF.
  - RF on distance to points could be applied to phylogeny. ## Using genus as categorical variable.

```
genus_dummy <- dummyVars(~ MSW05_Genus, data = p)
genus_dummy_data <- data.frame(predict(genus_dummy, newdata = p))

genus_data <- cbind(p_impute, genus_dummy_data)



rf_gr_gen <- expand.grid(mtry = c(5, 20, 30, 100, 300, 500), splitrule = 'variance', min.node.size = c(5, 10,
m3_rf_gen <- train(y ~ ., data = genus_data, method = 'ranger', tuneGrid = rf_gr_gen,
                   trControl = trcntrl, na.action = na.omit, importance = 'impurity',
                   save.memory = TRUE, num.trees = 1000)
```

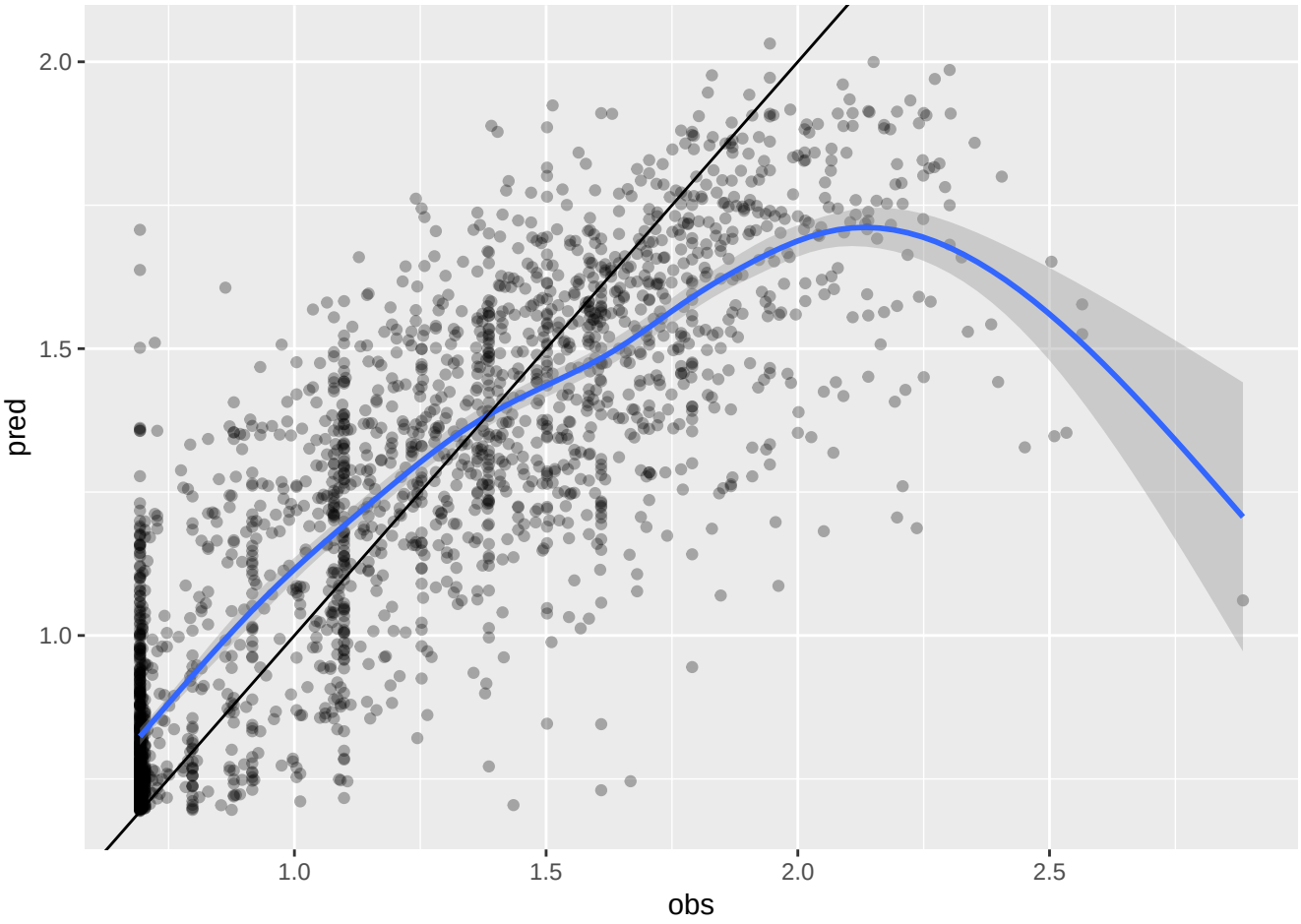
```
## Growing trees.. Progress: 38%. Estimated remaining time: 50 seconds.
## Growing trees.. Progress: 76%. Estimated remaining time: 19 seconds.
```

```
plot(m3_rf_gen)
```




```
plotCV(m3_rf_gen)
```

```
## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
```




```
m3_rf_gen
```

```
## Random Forest
##
## 2143 samples
## 1277 predictors
##
## No pre-processing
## Resampling: Bootstrapped (5 reps)
## Summary of sample sizes: 1714, 1715, 1714, 1715, 1714
## Resampling results across tuning parameters:
##
##   mtry  min.node.size  RMSE       Rsquared   MAE
##     5    5             0.3975884  0.5200278  0.3385923
##     5   10             0.3973934  0.5146602  0.3383181
##     5   20             0.3974637  0.5194522  0.3385134
##     5   50             0.3967874  0.5226459  0.3378351
##    20    5             0.3080060  0.6052501  0.2482522
##    20   10             0.3084312  0.6036814  0.2486763
##    20   20             0.3090979  0.6013703  0.2491830
##    20   50             0.3109547  0.5965261  0.2508497
##    30    5             0.2913776  0.6320828  0.2309635
##    30   10             0.2916158  0.6313681  0.2312531
##    30   20             0.2937845  0.6257520  0.2330478
##    30   50             0.2971199  0.6184921  0.2363593
##   100    5             0.2652209  0.6761404  0.2016485
##   100   10             0.2663579  0.6739501  0.2031777
##   100   20             0.2698517  0.6664558  0.2067950
##   100   50             0.2788782  0.6464537  0.2160755
##   300    5             0.2549070  0.6935480  0.1888755
```

```
##   300   10             0.2556478  0.6922447  0.1898970
##   300   20             0.2577598  0.6876857  0.1925412
##   300   50             0.2650015  0.6716487  0.1999991
##   500    5             0.2518618  0.6982343  0.1843303
##   500   10             0.2522184  0.6975714  0.1847423
##   500   20             0.2540926  0.6934045  0.1870148
##   500   50             0.2595860  0.6814795  0.1931563
##
## Tuning parameter 'splitrule' was held constant at a value of variance
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were mtry = 500, splitrule =
##  variance and min.node.size = 5.
```

```
m3_rf_gen$results$Rsquared %>% max
```

```
## [1] 0.6982343
```

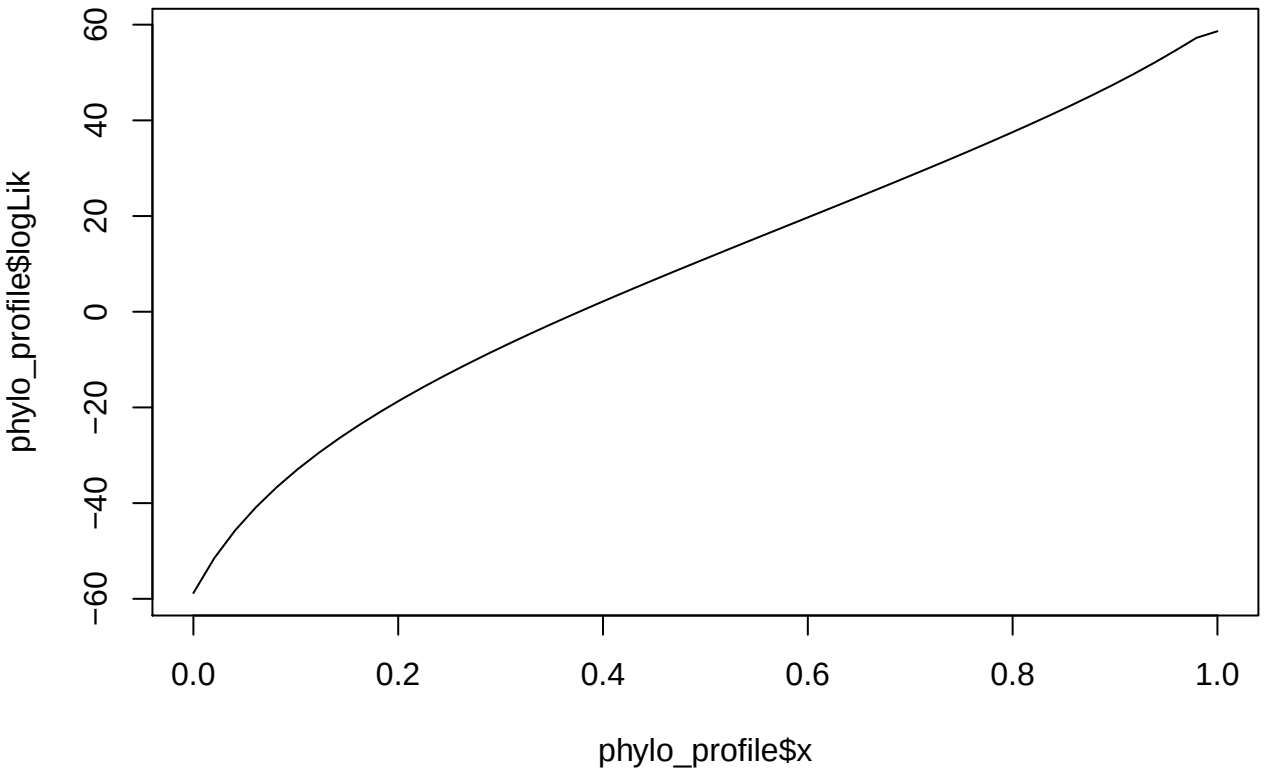
PGLS phylogenetic regression

Fit a standard pylogenetic regression with caper so we can check the later INLA models are reasonable.

```
comp_data <- comparative.data(tree, cbind(p_impute, MSW05_Binomial = p$MSW05_Binomial)[1:200, ], 'MSW05_Binomi

# Model will not run without log transforming.
apriori_formula_phylo <- y ~ X5.1_AdultBodyMass_g + X3.1_AgeatFirstBirth_d + X18.1_BasalMetRate_mLO2hr +
                             X9.1_GestationLen_d + X16.1_LittersPerYear + X17.1_MaxLongevity_m


m0_pglm <- pgls(apriori_formula_phylo, data = comp_data)

m0_pglm
```

```
##
## Call:
## pgls(formula = apriori_formula_phylo, data = comp_data)
##
## Coefficients:
##               (Intercept)       X5.1_AdultBodyMass_g
##                 1.176e+00                 -1.109e-02
##    X3.1_AgeatFirstBirth_d  X18.1_BasalMetRate_mLO2hr
##                -1.193e-05                  2.628e-02
##       X9.1_GestationLen_d       X16.1_LittersPerYear
##                -3.959e-02                  1.030e-02
##      X17.1_MaxLongevity_m
##                 1.123e-02
```

```
phylo_profile <- pgls.profile(m0_pglm)

plot(phylo_profile$logLik ~ phylo_profile$x, type = 'l')
```




```
nspp <- length(comp_data$phy$tip.label)
Vphy <- ape::vcv.phylo(comp_data$phy)
Vphy <- solve(Vphy)

order <- match(p$MSW05_Binomial[1:200], colnames(Vphy))
Vphy <- Vphy[order, order] # same order as species levels

# Decide a decent prior.
#  Want it to be considerably less than the sd of residuals from fixed effects model.
sd(m0_lm$finalModel$residuals)
```

```
## [1] 0.3698553
```

```
hyper.prior <- list(prec = list(prior="pc.prec", param = c(0.01, 0.00001)))

apriori_form_inla <- y ~ X5.1_AdultBodyMass_g + X3.1_AgeatFirstBirth_d + X18.1_BasalMetRate_mLO2hr +
                         X9.1_GestationLen_d + X16.1_LittersPerYear + X17.1_MaxLongevity_m +
                         f(phylo, model = 'generic0', Cmatrix = Vphy, hyper = hyper.prior)



m0_inla_comp <- inla(apriori_form_inla, data = cbind(p_impute[1:200, ], phylo = 1:200), control.predictor = li

# autoplot(m0_inla_comp)

m0_inla_comp$summary.fixed
```

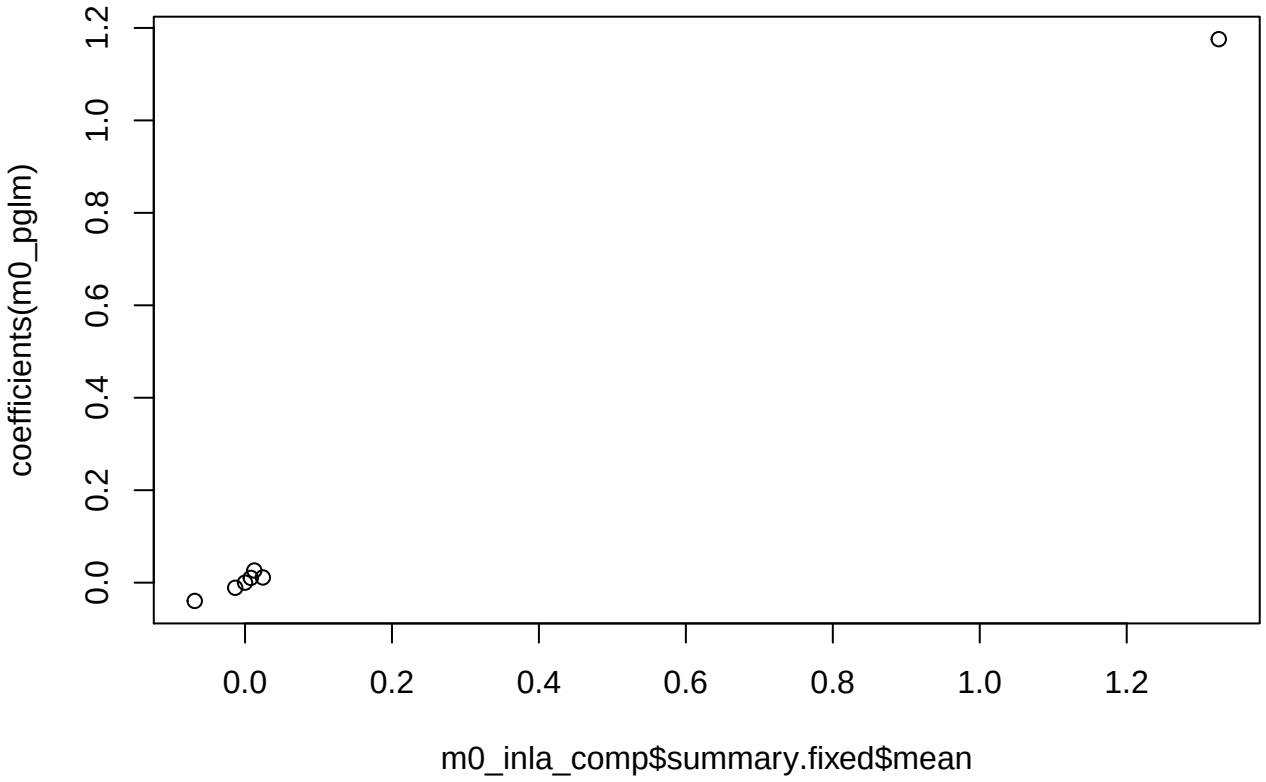
```
##                                 mean           sd    0.025quant
## (Intercept)                1.325296e+00 2.623426e-01  8.063124e-01
## X5.1_AdultBodyMass_g      -1.335263e-02 1.058011e-02 -3.413838e-02
## X3.1_AgeatFirstBirth_d    -1.540641e-05 2.714377e-05 -6.924512e-05
## X18.1_BasalMetRate_mLO2hr  1.265097e-02 1.455241e-02 -1.709562e-02
## X9.1_GestationLen_d       -6.843786e-02 2.940687e-02 -1.276682e-01
## X16.1_LittersPerYear       7.859127e-03 1.611157e-02 -2.396073e-02
## X17.1_MaxLongevity_m       2.424826e-02 2.965359e-02 -3.366914e-02
##                               0.5quant    0.975quant          mode
```

```
## (Intercept)                1.326539e+00  1.837003e+00  1.329127e+00
## X5.1_AdultBodyMass_g      -1.335375e-02  7.418337e-03 -1.335526e-02
## X3.1_AgeatFirstBirth_d    -1.527497e-05  3.763627e-05 -1.502183e-05
## X18.1_BasalMetRate_mLO2hr  1.305871e-02  4.016189e-02  1.389145e-02
## X9.1_GestationLen_d       -6.792392e-02 -1.205832e-02 -6.687515e-02
## X16.1_LittersPerYear       7.908972e-03  3.936747e-02  8.006255e-03
## X17.1_MaxLongevity_m       2.411722e-02  8.283189e-02  2.386250e-02
##                                     kld
## (Intercept)                1.976098e-13
## X5.1_AdultBodyMass_g       3.858528e-13
## X3.1_AgeatFirstBirth_d     1.341333e-12
## X18.1_BasalMetRate_mLO2hr  1.201881e-11
## X9.1_GestationLen_d        6.401673e-13
## X16.1_LittersPerYear       1.027705e-12
## X17.1_MaxLongevity_m       1.213065e-12
```

```
m0_inla_comp$summary.hyperpar
```

```
##                                            mean       sd 0.025quant
## Precision for the Gaussian observations 290.8399 187.4009   99.06641
## Precision for phylo                     906.8918 155.4347  616.07146
##                                         0.5quant 0.975quant     mode
## Precision for the Gaussian observations 238.3625   787.0792 170.8831
## Precision for phylo                     904.3730  1222.1420 909.4108
```

```
plot(m0_inla_comp$summary.fixed$mean, coefficients(m0_pglm))
```




```
comp_data_full <- comparative.data(tree, cbind(p_impute, MSW05_Binomial = p$MSW05_Binomial), 'MSW05_Binomial')

# Code broadly copied from https://github.com/daijiang/phyr/blob/master/R/pglmm-utils.R#L54
nspp <- length(comp_data_full$phy$tip.label)
Vphy <- ape::vcv(comp_data_full$phy)
Vphy <- solve(Vphy)

order <- match(p$MSW05_Binomial, colnames(Vphy))
Vphy <- Vphy[order, order] # same order as species levels
```

```r
# fit full model

m0_inla_comp_full <- inla(apriori_form_inla, data = cbind(p_impute, phylo = 1:nrow(p_impute)),
                      control.predictor = list(compute = TRUE),
                      control.inla= list(strategy = "gaussian", int.strategy = "eb"))



m0_inla_comp_full$summary.fixed
```

```
##                                    mean           sd    0.025quant
## (Intercept)                1.490076e+00 2.407773e-01  1.017349e+00
## X5.1_AdultBodyMass_g      -1.599514e-02 5.103820e-03 -2.601566e-02
## X3.1_AgeatFirstBirth_d    -5.429982e-07 1.553478e-05 -3.104301e-05
## X18.1_BasalMetRate_mLO2hr  9.608507e-03 5.766556e-03 -1.713187e-03
## X9.1_GestationLen_d       -5.141640e-02 1.207399e-02 -7.512172e-02
## X16.1_LittersPerYear       1.432133e-02 5.780201e-03  2.972849e-03
## X17.1_MaxLongevity_m      -2.616186e-02 9.996875e-03 -4.578910e-02
##                                0.5quant    0.975quant          mode
## (Intercept)                1.490070e+00  1.962409e+00  1.490076e+00
## X5.1_AdultBodyMass_g      -1.599529e-02 -5.982988e-03 -1.599514e-02
## X3.1_AgeatFirstBirth_d    -5.434357e-07  2.993156e-05 -5.429982e-07
## X18.1_BasalMetRate_mLO2hr  9.608345e-03  2.092075e-02  9.608507e-03
## X9.1_GestationLen_d       -5.141674e-02 -2.773087e-02 -5.141640e-02
## X16.1_LittersPerYear       1.432117e-02  2.566034e-02  1.432133e-02
## X17.1_MaxLongevity_m      -2.616214e-02 -6.551004e-03 -2.616186e-02
##                                    kld
## (Intercept)               2.267975e-30
## X5.1_AdultBodyMass_g      0.000000e+00
## X3.1_AgeatFirstBirth_d    0.000000e+00
## X18.1_BasalMetRate_mLO2hr 1.972152e-31
## X9.1_GestationLen_d       5.423419e-31
## X16.1_LittersPerYear      0.000000e+00
## X17.1_MaxLongevity_m      3.944305e-31
```

```r
m0_inla_comp_full$summary.hyperpar
```

```
##                                          mean        sd 0.025quant
## Precision for the Gaussian observations  51.07758  3.845308   43.98966
## Precision for phylo                     698.17100 48.367376  607.33180
##                                         0.5quant 0.975quant      mode
## Precision for the Gaussian observations  50.9168   59.07455  50.58312
## Precision for phylo                     696.7450  797.44724 694.14836
```

```r
# cross validation
m0_inla_comp2 <- list()

for(f in 1:5){

  cv_data <- cbind(p_impute, phylo = 1:nrow(p_impute))

  # remove hold out data
  cv_data$y[folds[[f]]] <- NA

  m0_inla_comp2[[f]] <- inla(apriori_form_inla, data = cv_data,
                      control.predictor = list(compute = TRUE),
                      control.inla= list(strategy = "gaussian", int.strategy = "eb"))
```

```
}
```

```
# calc rmse and scatter plot

inla_apriori_cvdat <- data.frame(y = p_impute$y, predy = NA)

for(f in 1:5){
  inla_apriori_cvdat$predy[folds[[f]]] <- m0_inla_comp2[[f]]$summary.fitted.values$mean[folds[[f]]]
}


sqrt(mean((inla_apriori_cvdat$predy - inla_apriori_cvdat$y) ^ 2))
```

```
## [1] 0.242759
```

```
cor(inla_apriori_cvdat$predy, inla_apriori_cvdat$y)
```

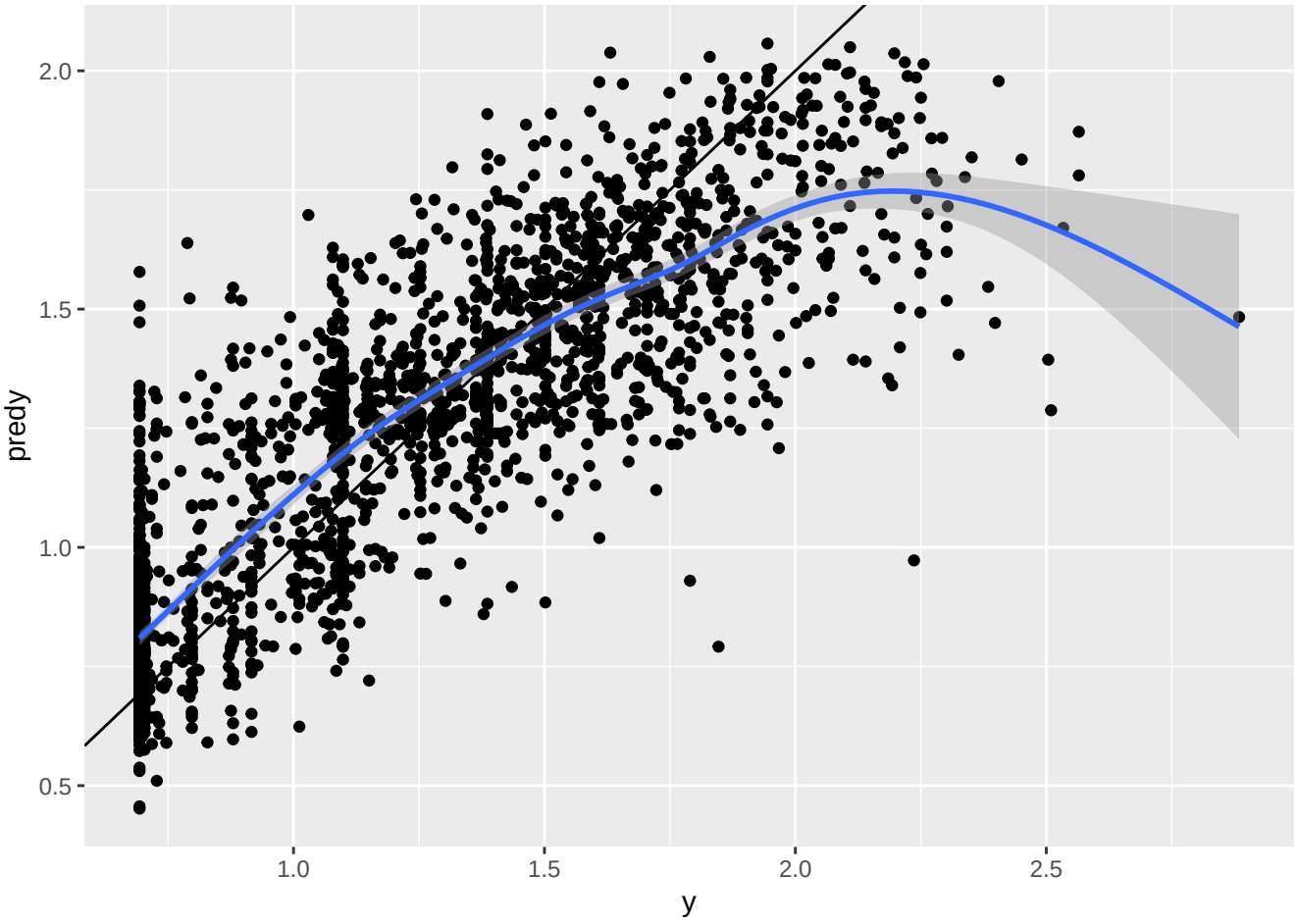
```
## [1] 0.8467217
```

```
lm(inla_apriori_cvdat$predy ~ inla_apriori_cvdat$y) %>% summary %>% `$`('r.squared')
```

```
## [1] 0.7169377
```

```
ggplot(inla_apriori_cvdat, aes(y, predy)) +
  geom_point() +
  #scale_y_continuous(limits = c(NA, 3)) +
  geom_abline(slope = 1, intercept = 0) +
  geom_smooth()
```

```
## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
```



Regularised linear model

```
# fit full model

enet_form_inla <- paste0('y ~ ', paste(names(p_impute %>% dplyr::select(- y)), collapse = ' + '),
                         ' + f(phylo, model = \'generic0\', Cmatrix = Vphy, hyper = hyper.prior)') %>% formul

# Select sd of fixed effect prior of 0.001. Gives us precision of 1e6.
m1_enet_inla_full <- inla(enet_form_inla, data = cbind(p_impute, phylo = 1:nrow(p_impute)),
                      control.predictor = list(compute = TRUE),
                      control.fixed = list(prec = 1e6),
                      control.inla= list(strategy = "gaussian", int.strategy = "eb"))



m1_enet_inla_full$summary.fixed
m1_enet_inla_full$summary.hyperpar
```

```
# cross validation
m1_enet_inla <- list()

for(f in 1:5){

  cv_data <- cbind(p_impute, phylo = 1:nrow(p_impute))

  # remove hold out data
  cv_data$y[folds[[f]]] <- NA

  m1_enet_inla[[f]] <- inla(enet_form_inla, data = cv_data,
                      control.predictor = list(compute = TRUE),
                      control.fixed = list(prec = 1e6),
                      control.inla= list(strategy = "gaussian", int.strategy = "eb"))

}
```

```
# calc rmse and scatter plot

inla_enet_cvdat <- data.frame(y = p_impute$y, predy = NA)

for(f in 1:5){
  inla_enet_cvdat$predy[folds[[f]]] <- m1_enet_inla[[f]]$summary.fitted.values$mean[folds[[f]]]
}


sqrt(mean((inla_enet_cvdat$predy - inla_enet_cvdat$y) ^ 2))
```

```
## [1] 0.2325696
```

```
cor(inla_enet_cvdat$predy, inla_enet_cvdat$y)
```

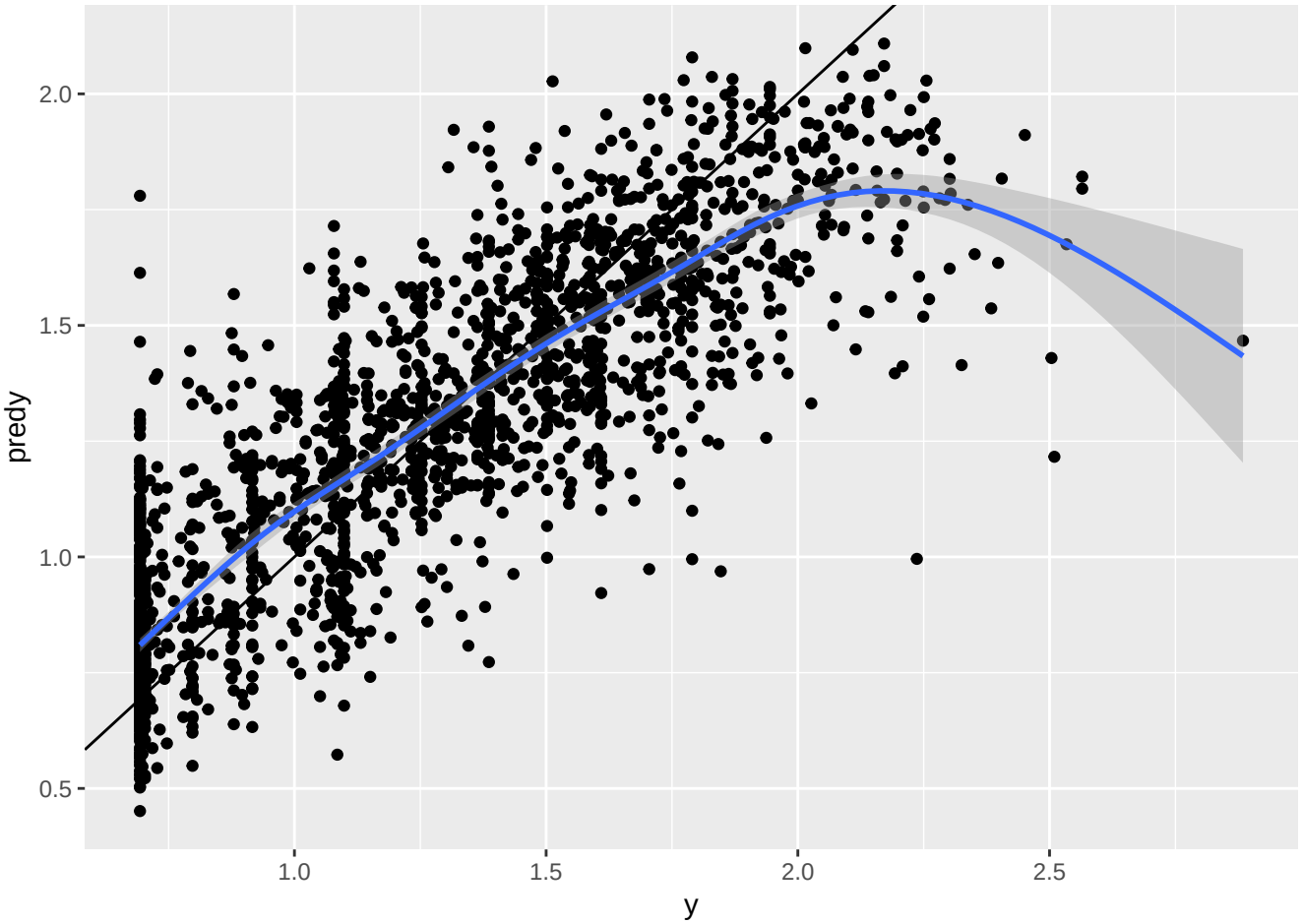
```
## [1] 0.8603091
```

```
lm(inla_enet_cvdat$predy ~ inla_enet_cvdat$y) %>% summary %>% `$`('r.squared')
```

```
## [1] 0.7401317
```

```
ggplot(inla_enet_cvdat, aes(y, predy)) +
  geom_point() +
  #scale_y_continuous(limits = c(NA, 3)) +
  geom_abline(slope = 1, intercept = 0) +
  geom_smooth()
```

```
## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
```




```
mlist <- list(m1_enet, m2_gp, m3_rf)

cv_preds_raw <- lapply(mlist, best_tune_preds)
cv_preds <- lapply(seq_along(cv_preds_raw), function (x) cv_preds_raw[[x]]$pred)
cv_preds <- do.call(cbind, cv_preds) %>% data.frame

# Put into correct order
cv_preds <- cv_preds[order(cv_preds_raw[[1]]$rowIndex), ]

names(cv_preds) <- c('enet', 'gp', 'rf')

cv_preds <- mutate(cv_preds, y = p_impute$y) # check order
cv_preds$phylo <- seq_len(nrow(cv_preds))

stacked_form <- y ~ 0 +
  f(enet, model='clinear', range=c(0, Inf), initial=0) +
  f(gp, model='clinear', range=c(0, Inf), initial=0) +
  f(rf, model='clinear', range=c(0, Inf), initial=0) +
  f(phylo, model = 'generic0', Cmatrix = Vphy, hyper = hyper.prior)
```

```
stacked_full <- inla(stacked_form, data = cv_preds,
                     control.predictor = list(compute = TRUE),
                     control.inla= list(strategy = "gaussian", int.strategy = "eb"))


stacked_full$summary.fixed
```

```
## data frame with 0 columns and 0 rows
```

```
stacked_full$summary.hyperpar
```

```
##                                                mean          sd
## Precision for the Gaussian observations   44.0704027  2.96503674
## Beta for enet                              0.1605476  0.02050353
## Beta for gp                                0.1835898  0.02345746
## Beta for rf                                0.3514981  0.03073841
## Precision for phylo                     1060.0785512 93.23983894
##                                          0.025quant     0.5quant
## Precision for the Gaussian observations  38.4920278   43.9863867
## Beta for enet                             0.1237593    0.1593646
## Beta for gp                               0.1417057    0.1821645
## Beta for rf                               0.2953634    0.3500297
## Precision for phylo                     890.1276376 1055.4593876
##                                          0.975quant         mode
## Precision for the Gaussian observations   50.1467747   43.8344459
## Beta for enet                              0.2042373    0.1571290
## Beta for gp                                0.2337631    0.1794077
## Beta for rf                                0.4159495    0.3470030
## Precision for phylo                     1255.8172631 1045.8258139
```

```
# cross validation

stacked_full2 <- list()

for(f in 1:5){

  cv_data <- cv_preds

  # remove hold out data
  cv_data$y[folds[[f]]] <- NA

  stacked_full2[[f]] <- inla(stacked_form, data = cv_data,
                      control.predictor = list(compute = TRUE),
                      control.inla= list(strategy = "gaussian", int.strategy = "eb"))

}
```

```
# calc rmse and scatter plot

stacked_cvdat <- data.frame(y = p_impute$y, predy = NA)

for(f in 1:5){
  stacked_cvdat$predy[folds[[f]]] <- stacked_full2[[f]]$summary.fitted.values$mean[folds[[f]]]
}


sqrt(mean((stacked_cvdat$predy - stacked_cvdat$y) ^ 2))
```

```
## [1] 0.2421599
```

```
cor(stacked_cvdat$predy, stacked_cvdat$y)
```

```
## [1] 0.8491472
```

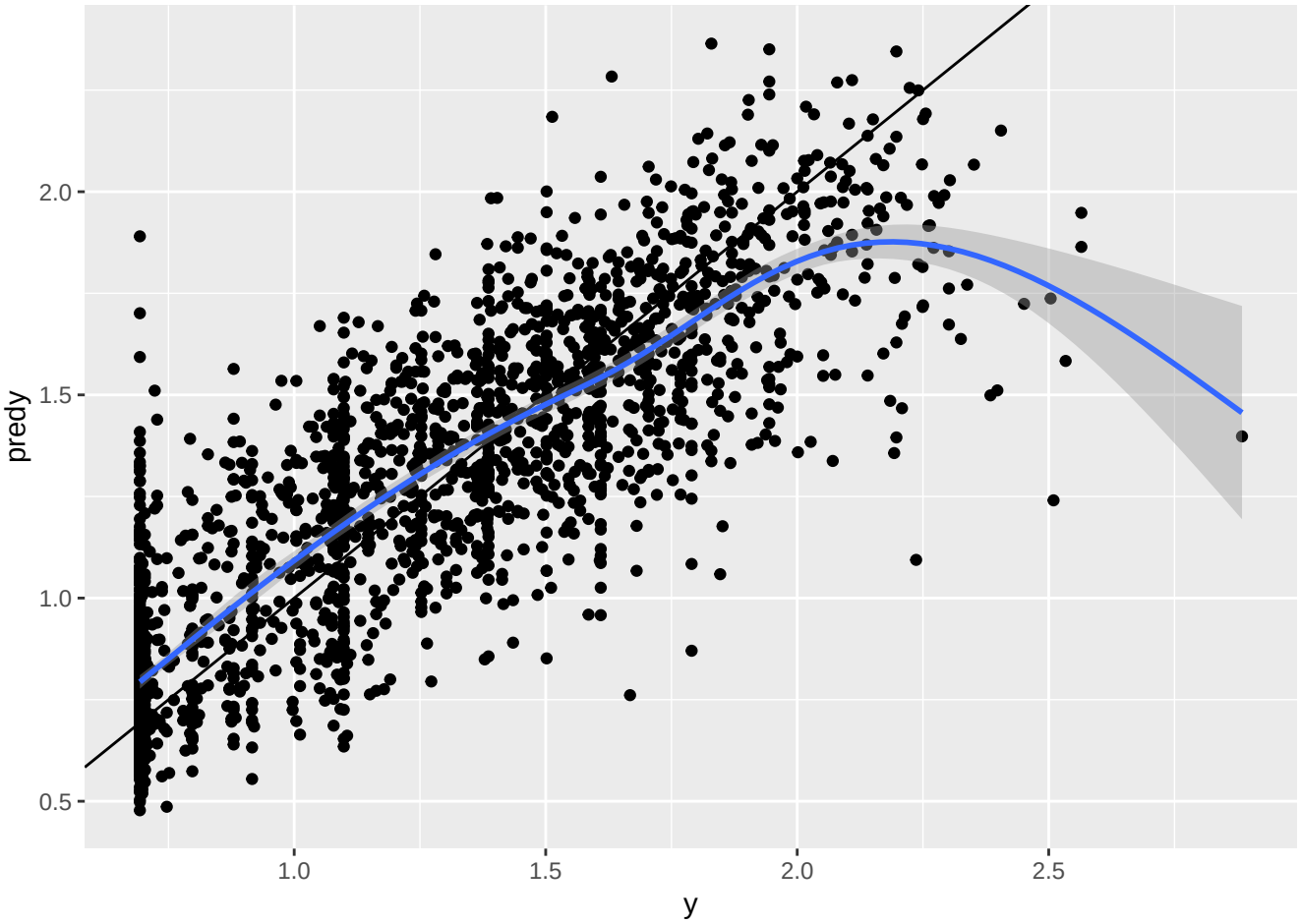
```
lm(stacked_cvdat$predy ~ stacked_cvdat$y) %>% summary %>% `$`('r.squared')
```

```
## [1] 0.721051
```

```
ggplot(stacked_cvdat, aes(y, predy)) +
  geom_point() +
  #scale_y_continuous(limits = c(NA, 3)) +
  geom_abline(slope = 1, intercept = 0) +
```

```
  geom_smooth()
```

```
## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
```

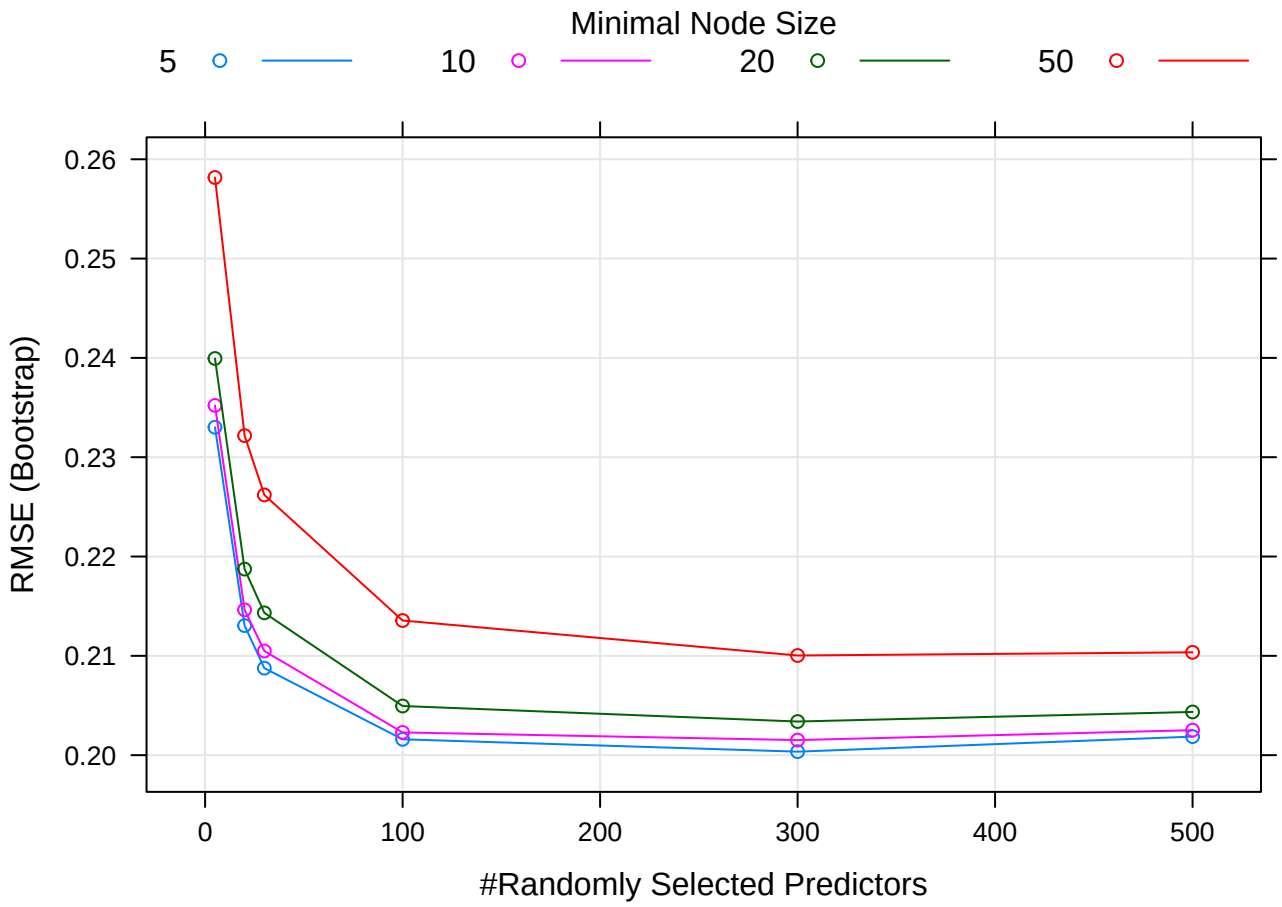


Using distance to each other as covariates

```
dist <- ape::cophenetic.phylo(comp_data_full$phy)
dist <- dist[order, order] # same order as species levels

dist_data <- cbind(p_impute, dist)

m3_rf_dist <- train(y ~ ., data = dist_data, method = 'ranger', tuneGrid = rf_gr_gen,
                    trControl = trcntrl, na.action = na.omit, importance = 'impurity',
                    save.memory = TRUE, num.trees = 1000)
```

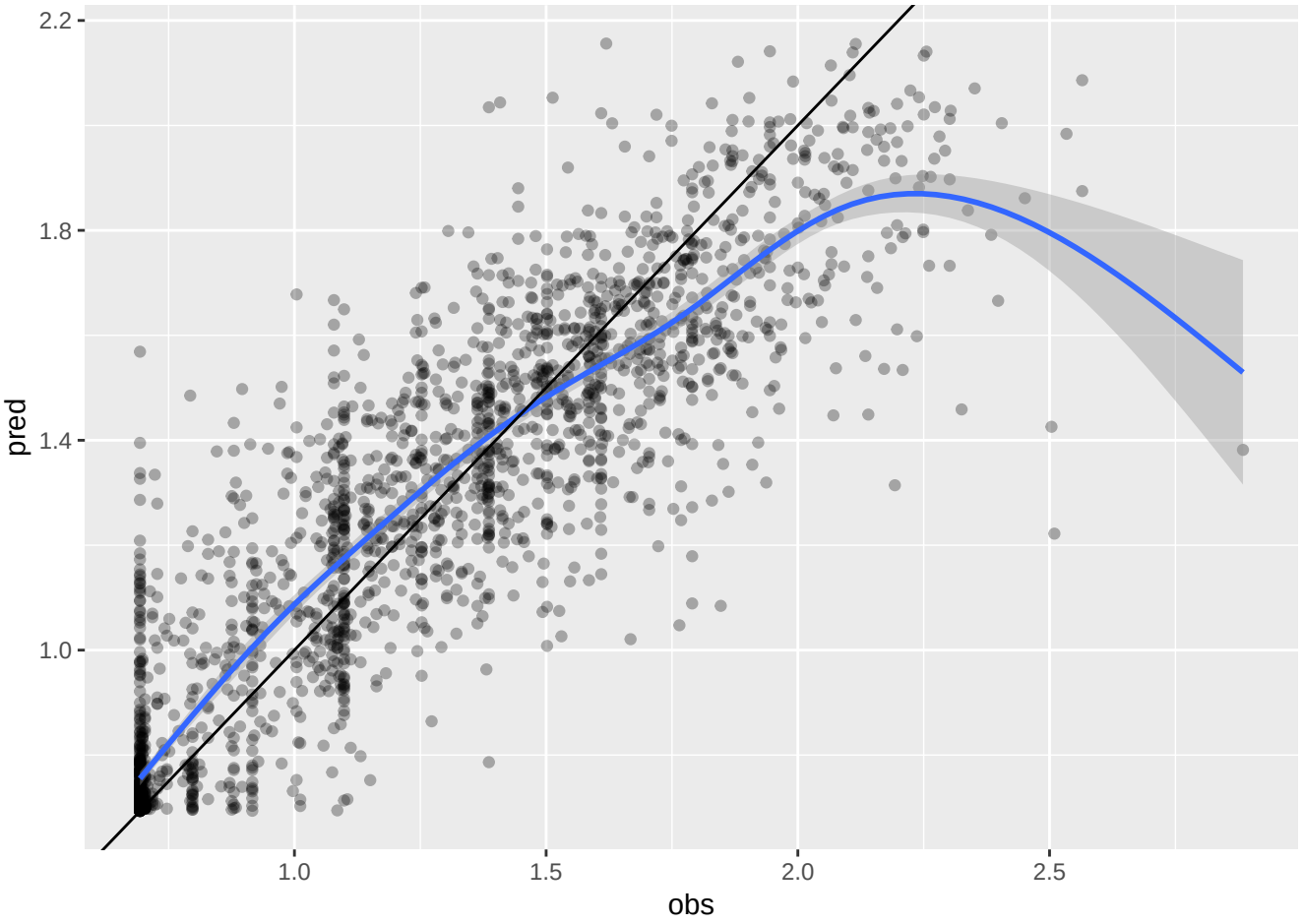
```
## Growing trees.. Progress: 19%. Estimated remaining time: 2 minutes, 16 seconds.
## Growing trees.. Progress: 39%. Estimated remaining time: 1 minute, 38 seconds.
## Growing trees.. Progress: 58%. Estimated remaining time: 1 minute, 6 seconds.
## Growing trees.. Progress: 78%. Estimated remaining time: 35 seconds.
## Growing trees.. Progress: 98%. Estimated remaining time: 3 seconds.
```

```
plot(m3_rf_dist)
```




```
plotCV(m3_rf_dist)
```

```
## `geom_smooth()` using method = 'gam' and formula 'y ~ s(x, bs = "cs")'
```




```
m3_rf_dist
```

```
## Random Forest
##
## 2143 samples
## 2190 predictors
##
## No pre-processing
## Resampling: Bootstrapped (5 reps)
## Summary of sample sizes: 1714, 1715, 1714, 1715, 1714
## Resampling results across tuning parameters:
##
##   mtry  min.node.size  RMSE       Rsquared   MAE
##     5    5             0.2330206  0.7387793  0.1633385
##     5   10             0.2352168  0.7342702  0.1658948
##     5   20             0.2399383  0.7246471  0.1712113
##     5   50             0.2581654  0.6830884  0.1876714
##    20    5             0.2130462  0.7810381  0.1451401
##    20   10             0.2146317  0.7779104  0.1472152
##    20   20             0.2187356  0.7698582  0.1522700
##    20   50             0.2321760  0.7426681  0.1653027
##    30    5             0.2087589  0.7898324  0.1420413
##    30   10             0.2104853  0.7865754  0.1445030
##    30   20             0.2143276  0.7790480  0.1490468
##    30   50             0.2262028  0.7554625  0.1603118
##   100    5             0.2015960  0.8042570  0.1382527
##   100   10             0.2022899  0.8030139  0.1396084
##   100   20             0.2049504  0.7979310  0.1422218
##   100   50             0.2135562  0.7812562  0.1502735
##   300    5             0.2003519  0.8069550  0.1378101
```

```
##   300   10             0.2015170  0.8048209  0.1388489
##   300   20             0.2033859  0.8012281  0.1410010
##   300   50             0.2100360  0.7884138  0.1471126
##   500    5             0.2018675  0.8042896  0.1391457
##   500   10             0.2025135  0.8032176  0.1399057
##   500   20             0.2043507  0.7996878  0.1417907
##   500   50             0.2103543  0.7883724  0.1477301
##
## Tuning parameter 'splitrule' was held constant at a value of variance
## RMSE was used to select the optimal model using the smallest value.
## The final values used for the model were mtry = 300, splitrule =
##  variance and min.node.size = 5.
```

```
m3_rf_dist$results$Rsquared %>% max
```

```
## [1] 0.806955
```

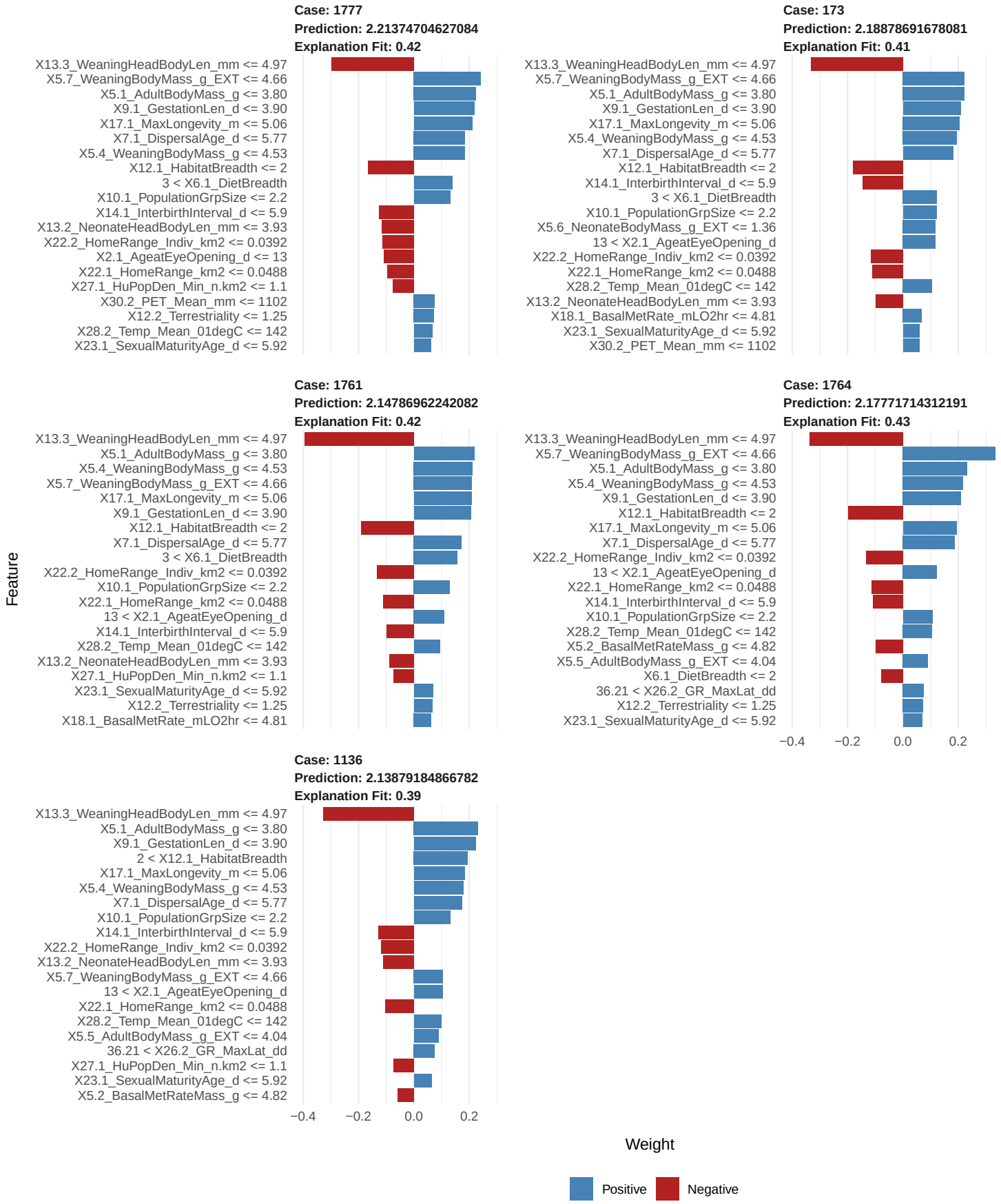
Point level understanding

- understand individual points
  - lime

```
# Explain Tenrec ecaudatus. Largest litter size. And other large litters
l1 <- pred_head(m1_enet)
l2 <- pred_head(m2_gp)
l3 <- pred_head(m3_rf)


m1_lime <- lime(p_impute, m1_enet)
```

```
## Warning: X12.2_Terrestriality does not contain enough variance to use quantile binning. Using standard binn
```

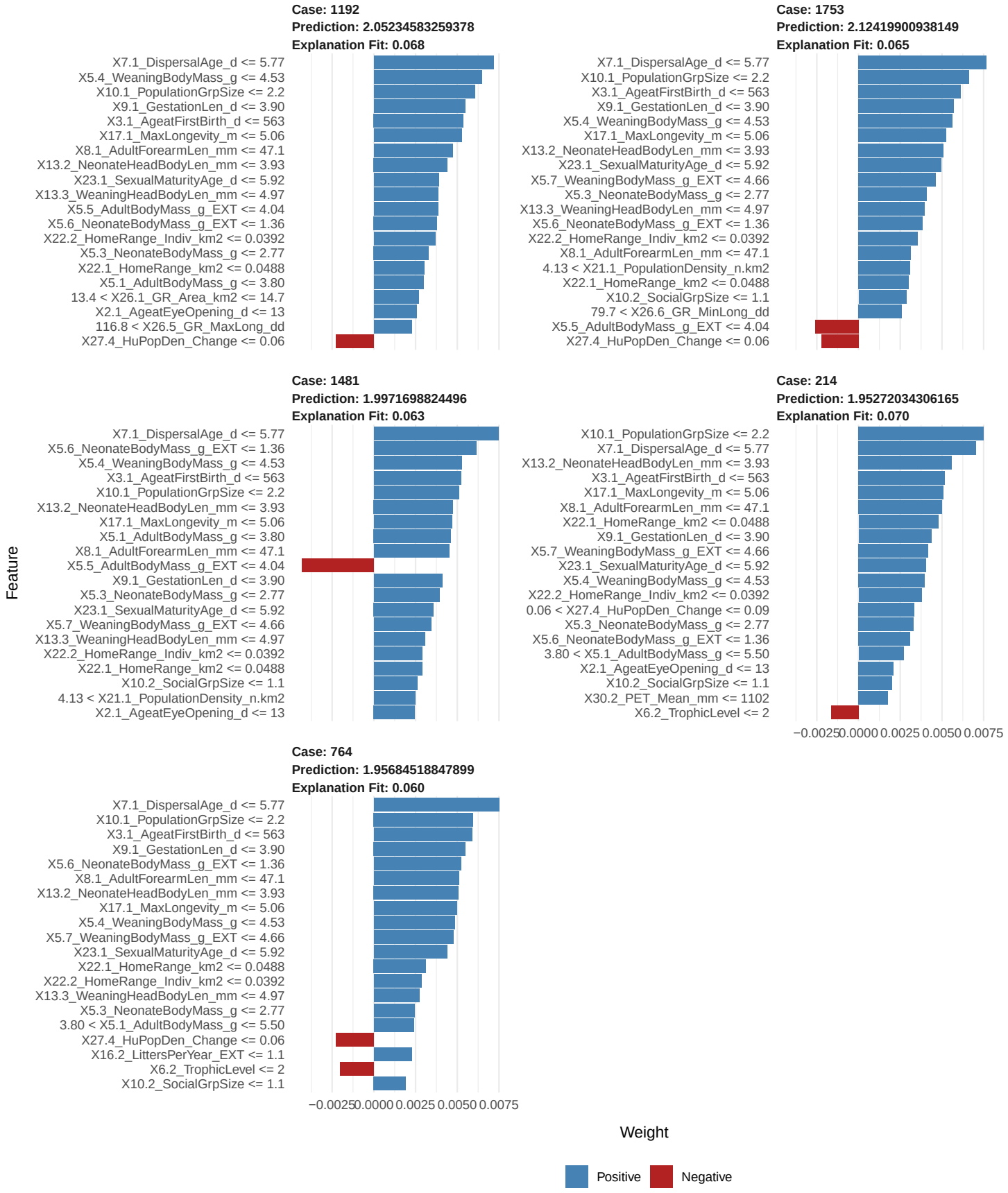
```
m1_explain <- explain(p_impute[l1, ], m1_lime, n_features = 20, feature_select = 'auto')

plot_features(m1_explain)
```




```
m2_lime <- lime(p_impute, m2_gp)
```

```
## Warning: X12.2_Terrestriality does not contain enough variance to use quantile binning. Using standard binn
```

```
m2_explain <- explain(p_impute[l2, ], m2_lime, n_features = 20, feature_select = 'auto')

plot_features(m2_explain)
```



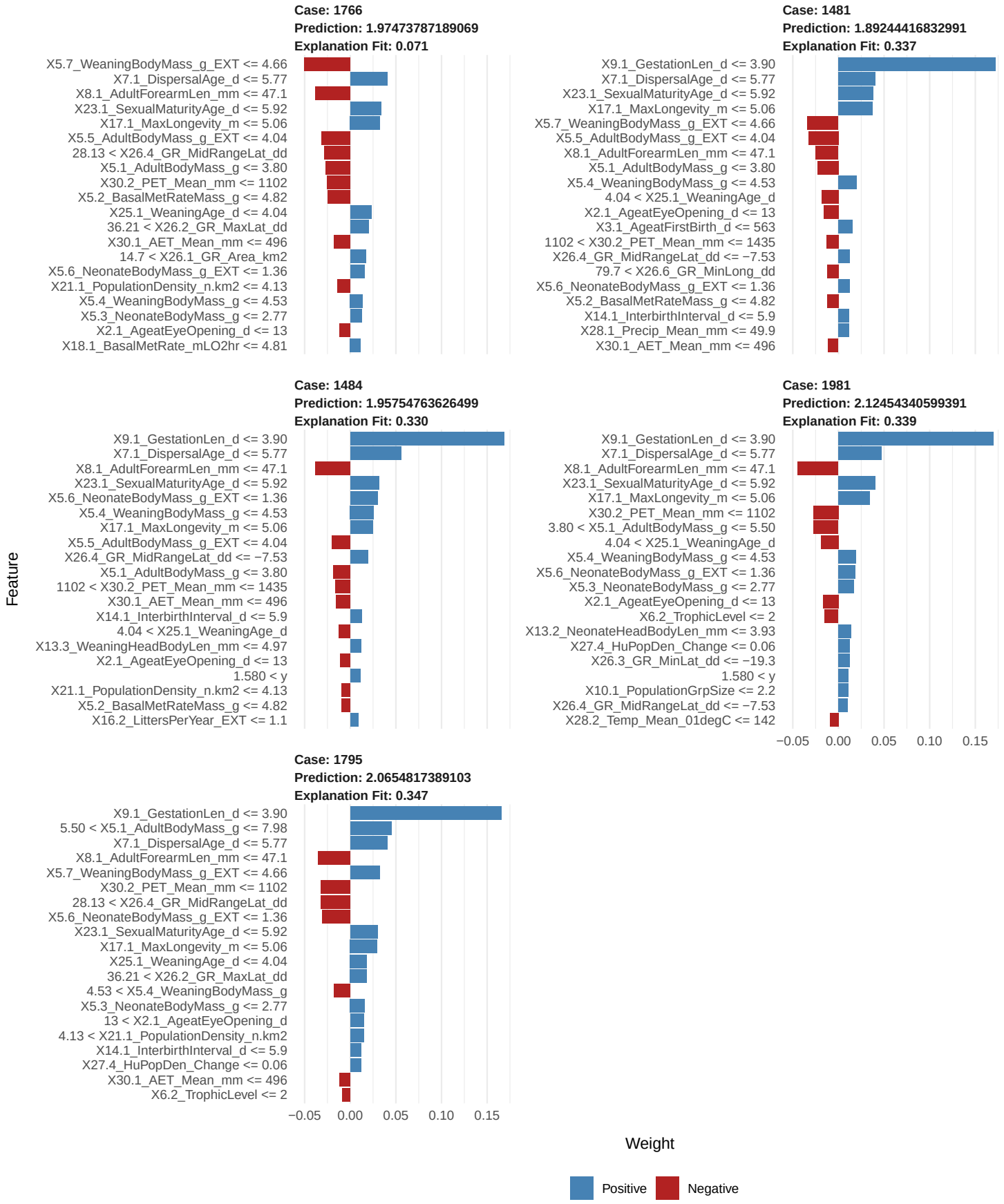
```
m3_lime <- lime(p_impute, m3_rf)
```

```
## Warning: X12.2_Terrestriality does not contain enough variance to use quantile binning. Using standard binn
```

```
m3_explain <- explain(p_impute[13, ], m3_lime, n_features = 20, feature_select = 'auto')
```

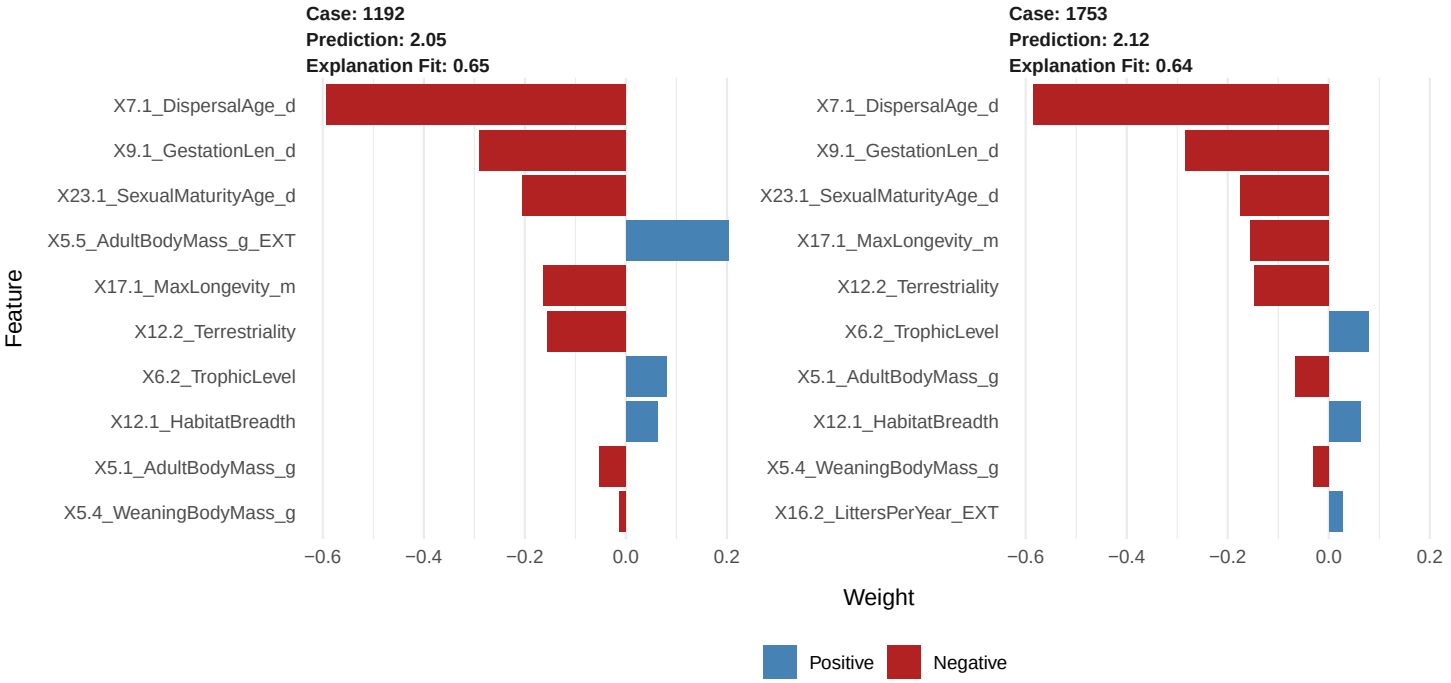
```
## Warning in predict.ranger.forest(forest, data, predict.all, num.trees, type, : Forest grown in ranger versi
```

```
plot_features(m3_explain)
```




```
l2 <- pred_head(m2_gp, 2)
l3 <- pred_head(m3_rf, 2)


m2_lime2 <- lime(p_impute, m2_gp, bin_continuous = FALSE, quantile_bins = FALSE)
```

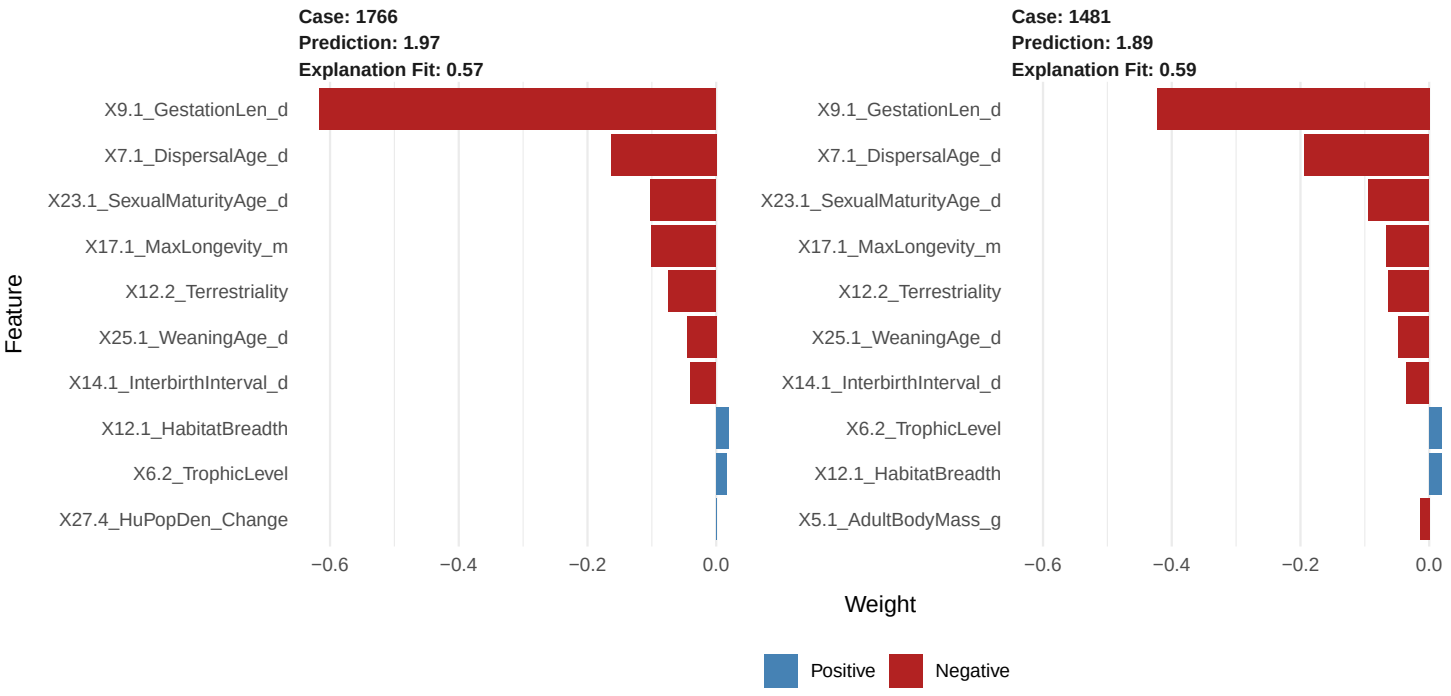
```
m2_explain2 <- explain(p_impute[l2, ], m2_lime2, n_features = 10, feature_select = 'auto')
m2_explain2$prediction <- round(m2_explain2$prediction, 2)

plot_features(m2_explain2)
```




```
m3_lime2 <- lime(p_impute, m3_rf, bin_continuous = FALSE, quantile_bins = FALSE)

m3_explain2 <- explain(p_impute[l3, ], m3_lime2, n_features = 10, feature_select = 'auto')
```

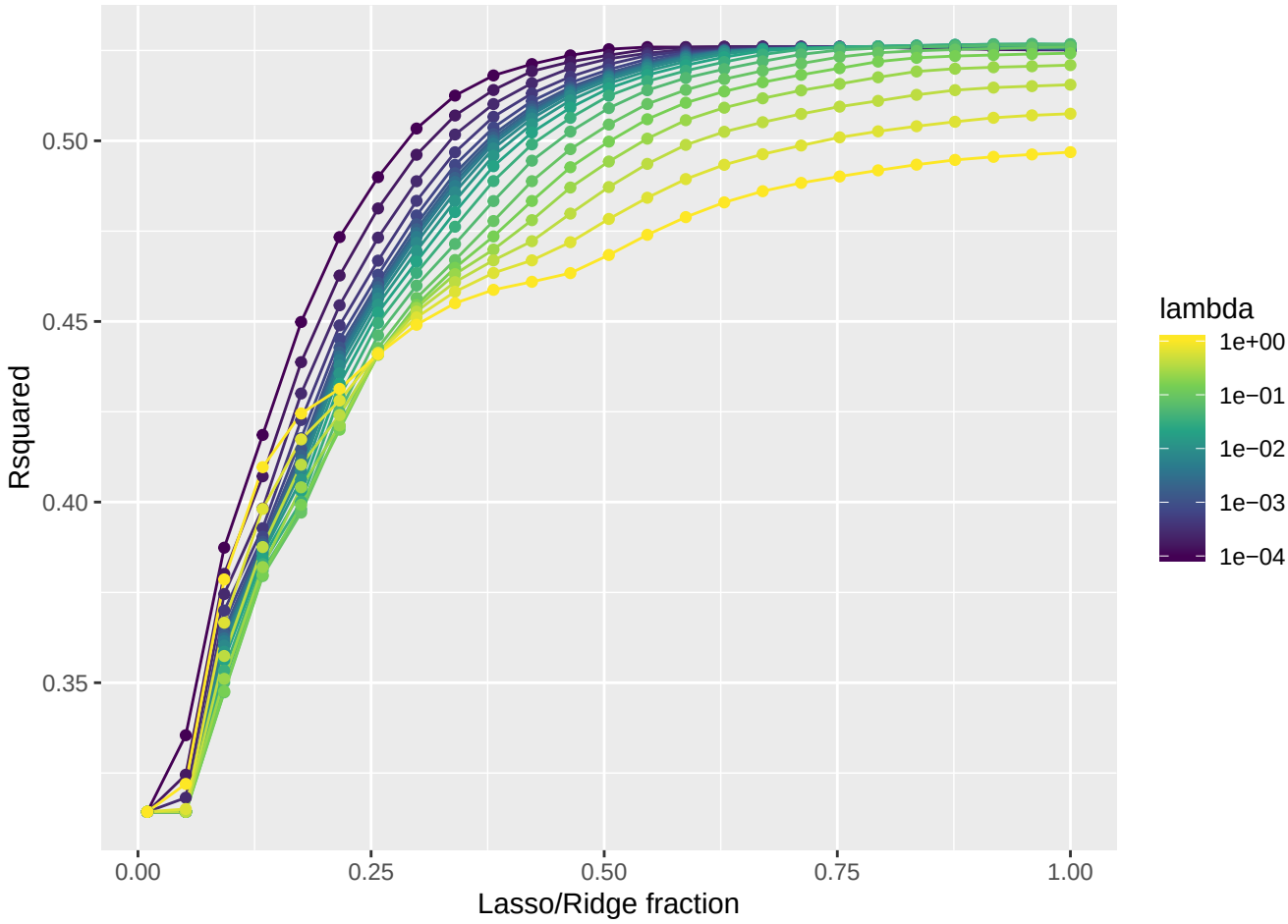
```
## Warning in predict.ranger.forest(forest, data, predict.all, num.trees, type, : Forest grown in ranger versi
```

```
m3_explain2$prediction <- round(m3_explain2$prediction, 2)
plot_features(m3_explain2)
```

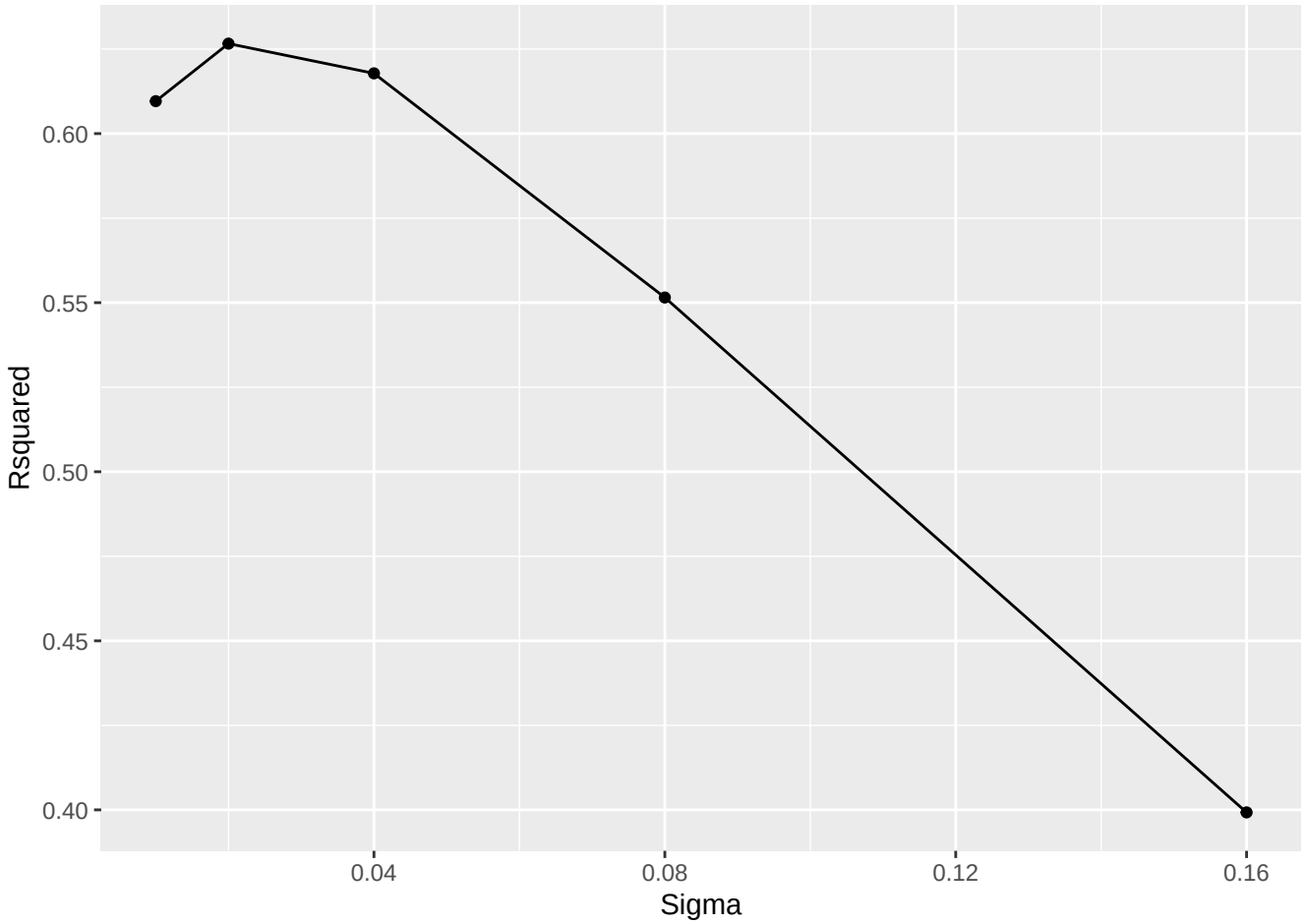



```
m1_enet$results %>%
  ggplot(aes(fraction, Rsquared, colour = lambda, group = factor(lambda))) +
    geom_line() +
```

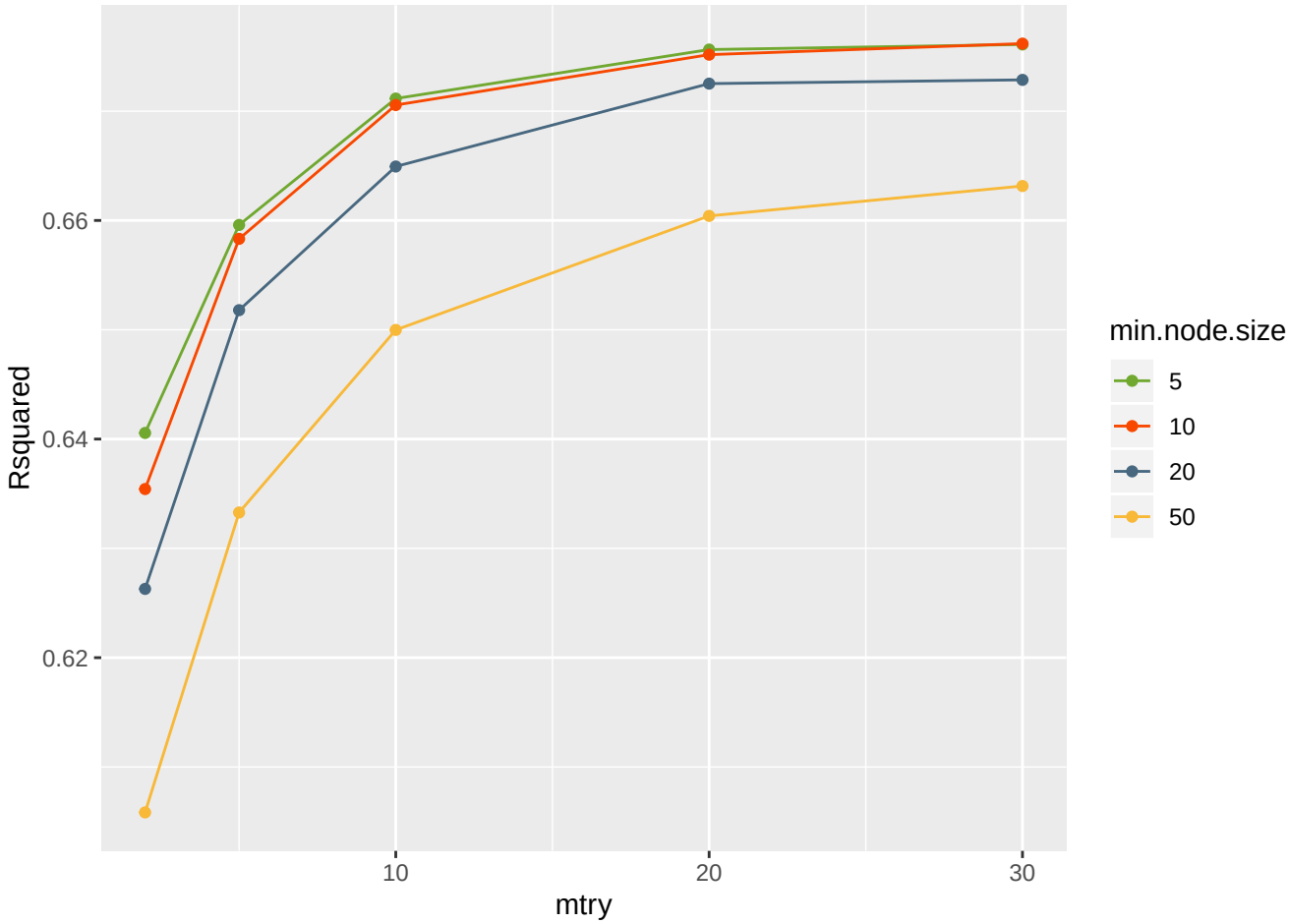
```
    geom_point() +
    scale_color_viridis_c(trans = 'log10') +
    xlab('Lasso/Ridge fraction')
```



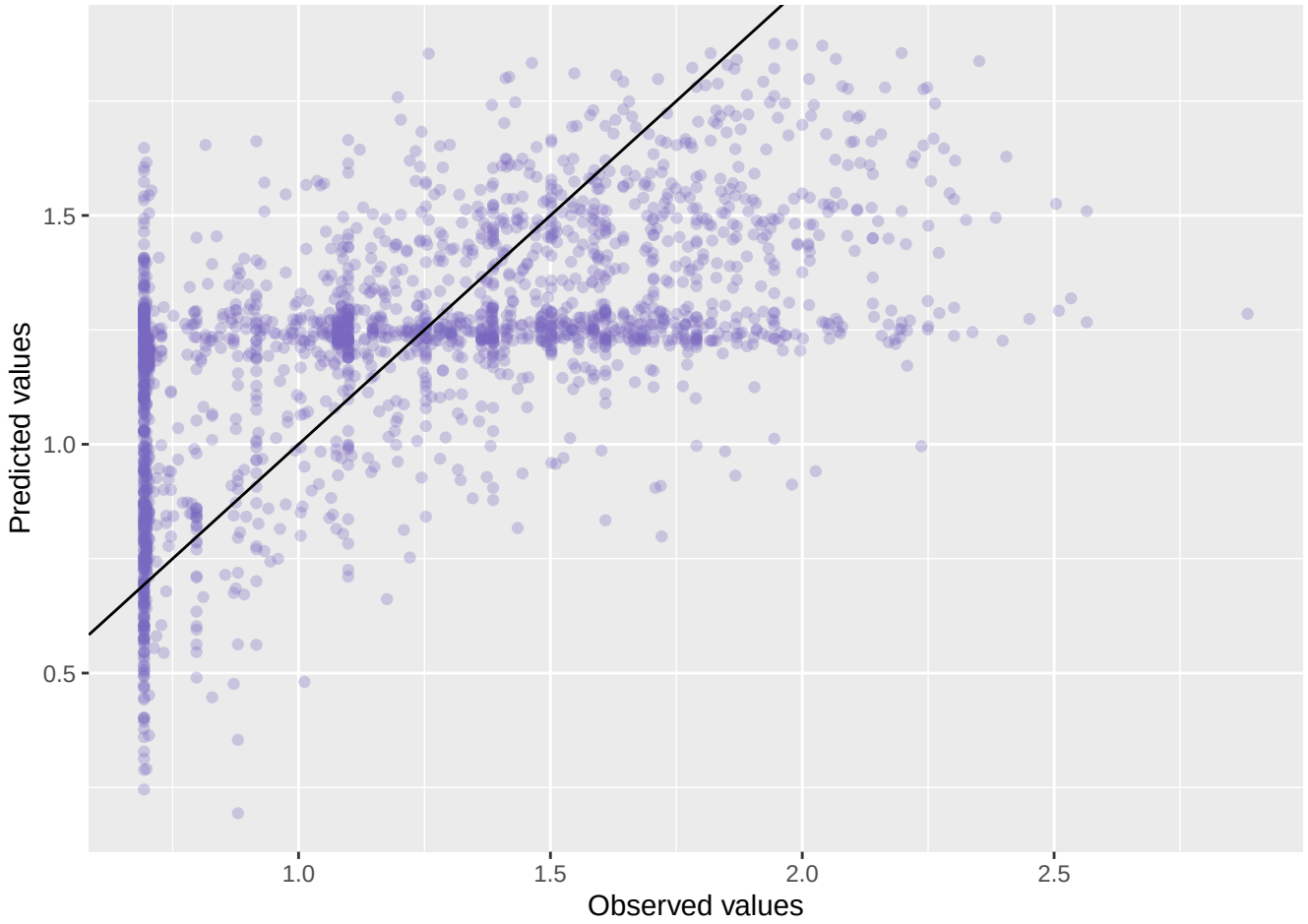

```
m2_gp$results %>%
  ggplot(aes(sigma, Rsquared)) +
    geom_line() +
    geom_point() +
    xlab('Sigma')
```



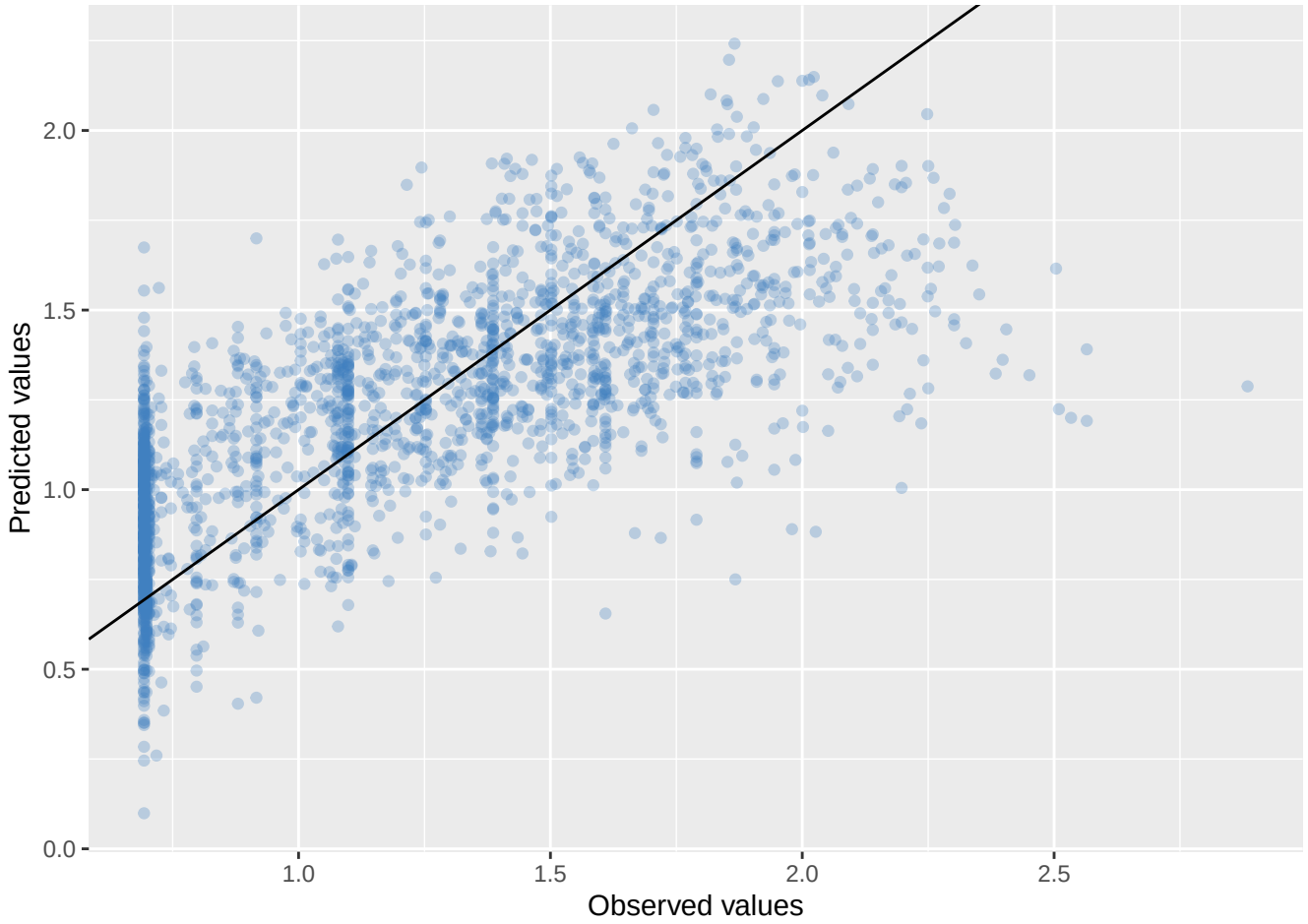

```
m3_rf$results %>%
  ggplot(aes(mtry, Rsquared, colour = factor(min.node.size), group = factor(min.node.size))) +
    geom_line() +
    geom_point() +
    scale_colour_poke(pokemon = 'oddish', spread = 4) +
    xlab('mtry') +
    labs(colour = 'min.node.size')
```



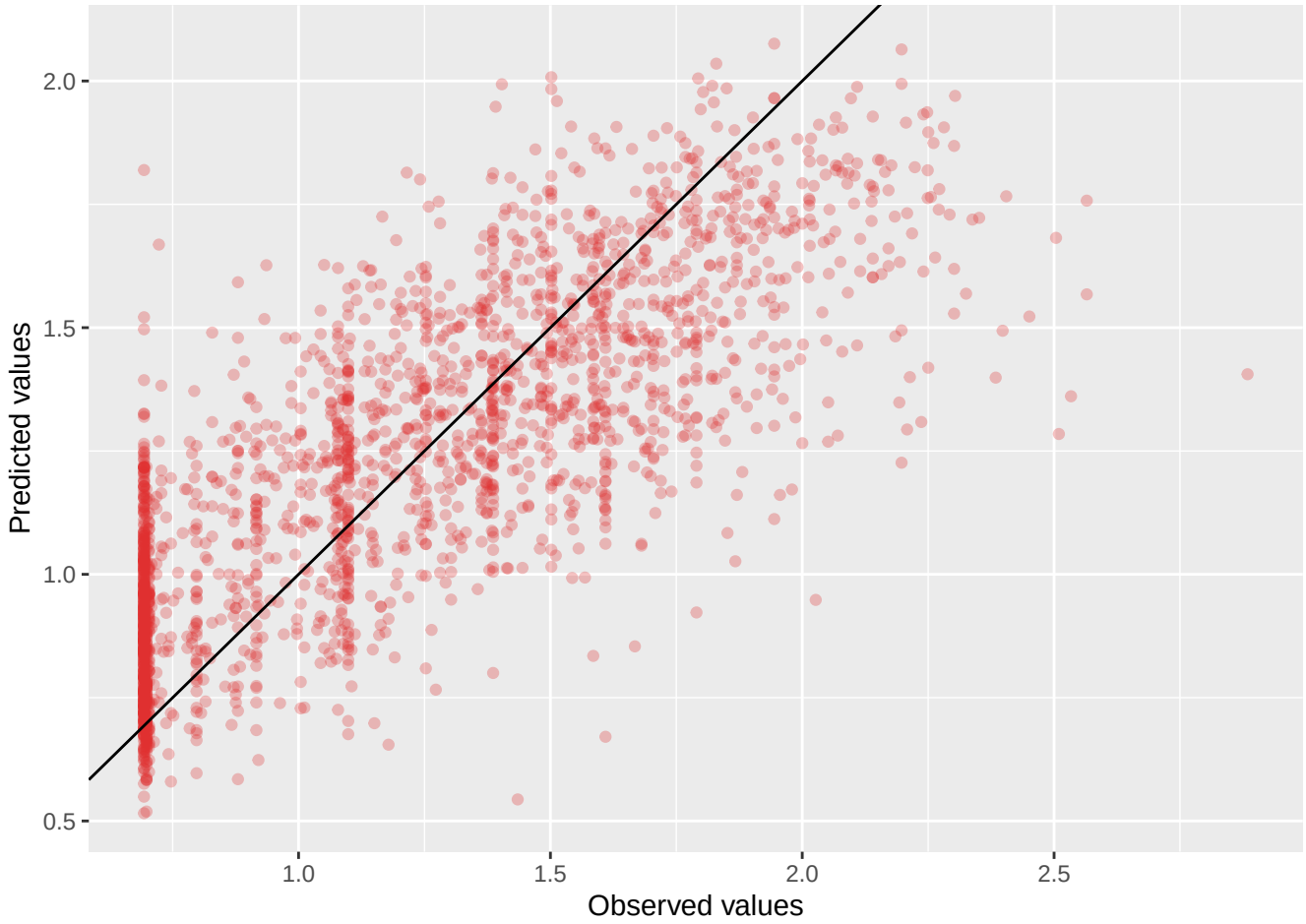

```
plotCV(m0_lm, smooth = FALSE, print = FALSE) +
  scale_colour_poke(pokemon = 'wartortle') +
  xlab('Observed values') +
  ylab('Predicted values')
```



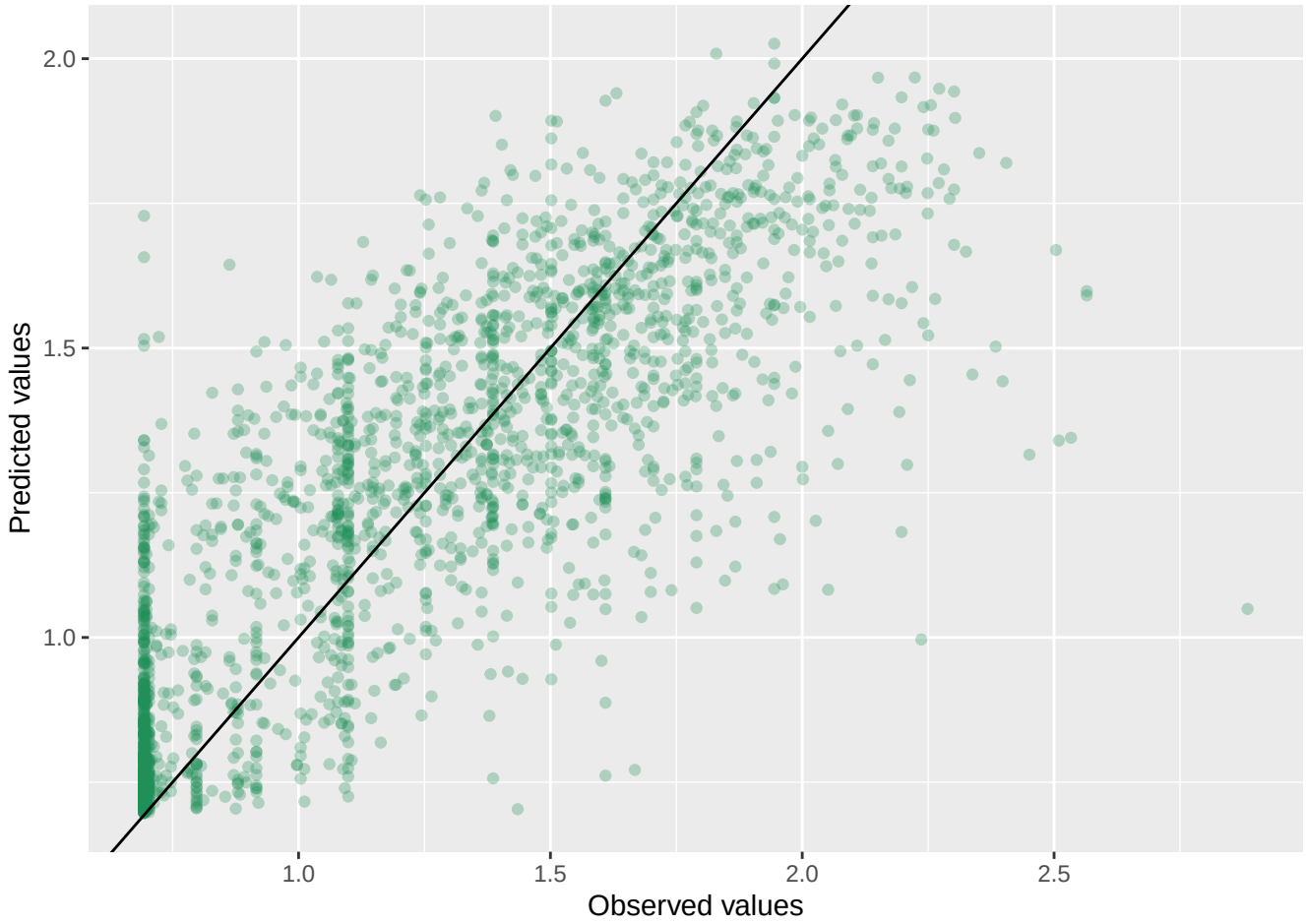

```
plotCV(m1_enet, smooth = FALSE, print = FALSE) +
  scale_colour_poke(pokemon = 'blastoise')+
  xlab('Observed values') +
  ylab('Predicted values')
```




```
plotCV(m2_gp, smooth = FALSE, print = FALSE) +
  scale_colour_poke(pokemon = 'parasect')+
  xlab('Observed values') +
  ylab('Predicted values')
```

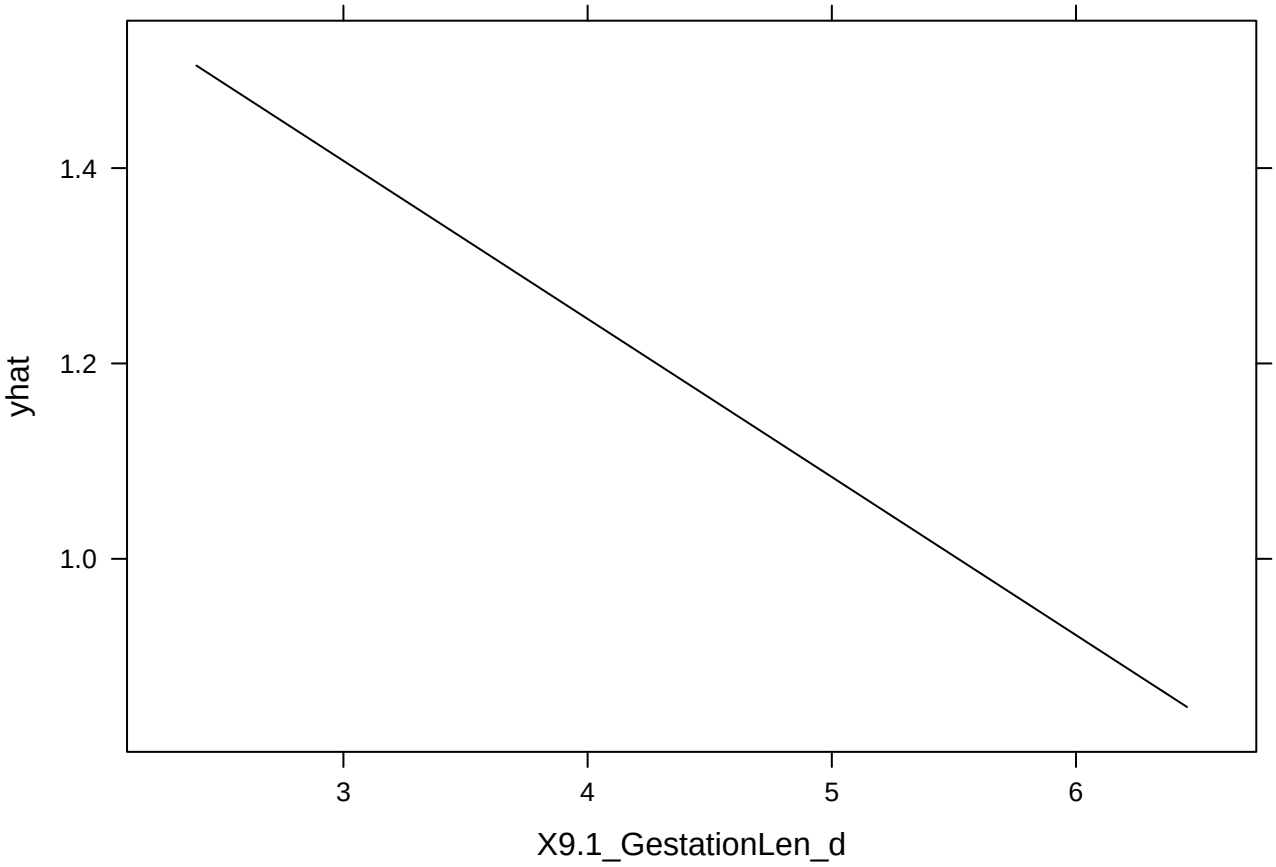



```
plotCV(m3_rf, smooth = FALSE, print = FALSE) +
  scale_colour_poke(pokemon = 'venusaur')+
  xlab('Observed values') +
  ylab('Predicted values')
```




```
partial(m1_enet,
        pred.var = c('X9.1_GestationLen_d'),
        parallel = TRUE, plot = TRUE)
```

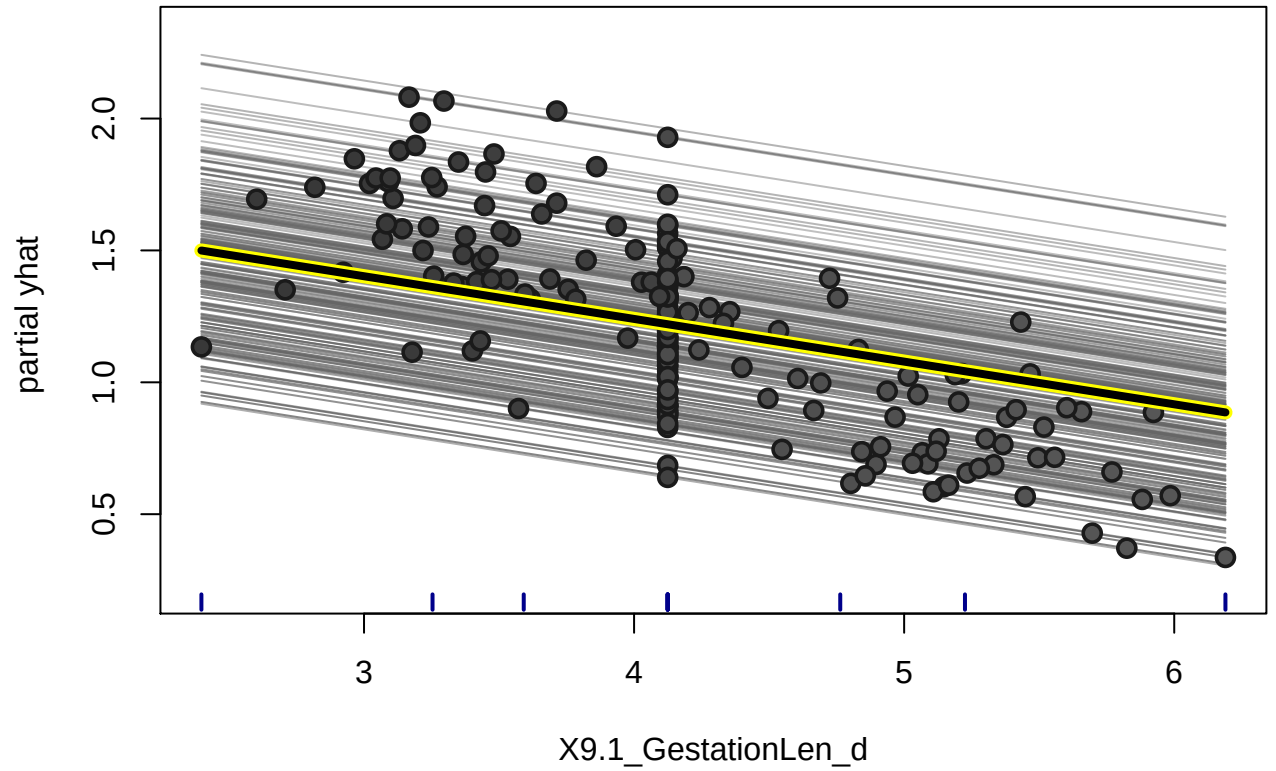
```
## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'

## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'
```




```
m1_enet_ice <- ice(m1_enet, p_impute, p_impute$y, 'X9.1_GestationLen_d', frac_to_build = 0.1)
```

```
## ................................................................................................
```

```
plot(m1_enet_ice)
```

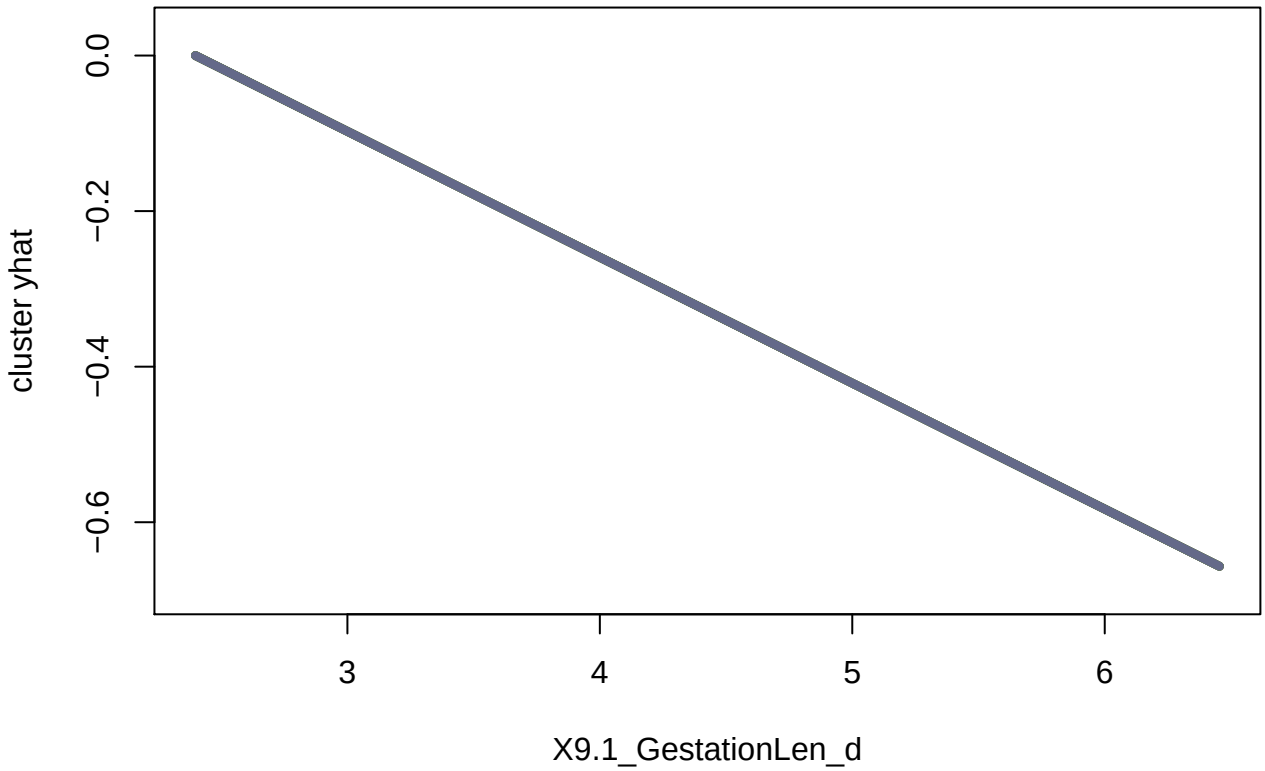



```
m1_enet_ice_c <- ice(m1_enet, p_impute, p_impute$y, 'X9.1_GestationLen_d')
```

```
## ................................................................................................
```

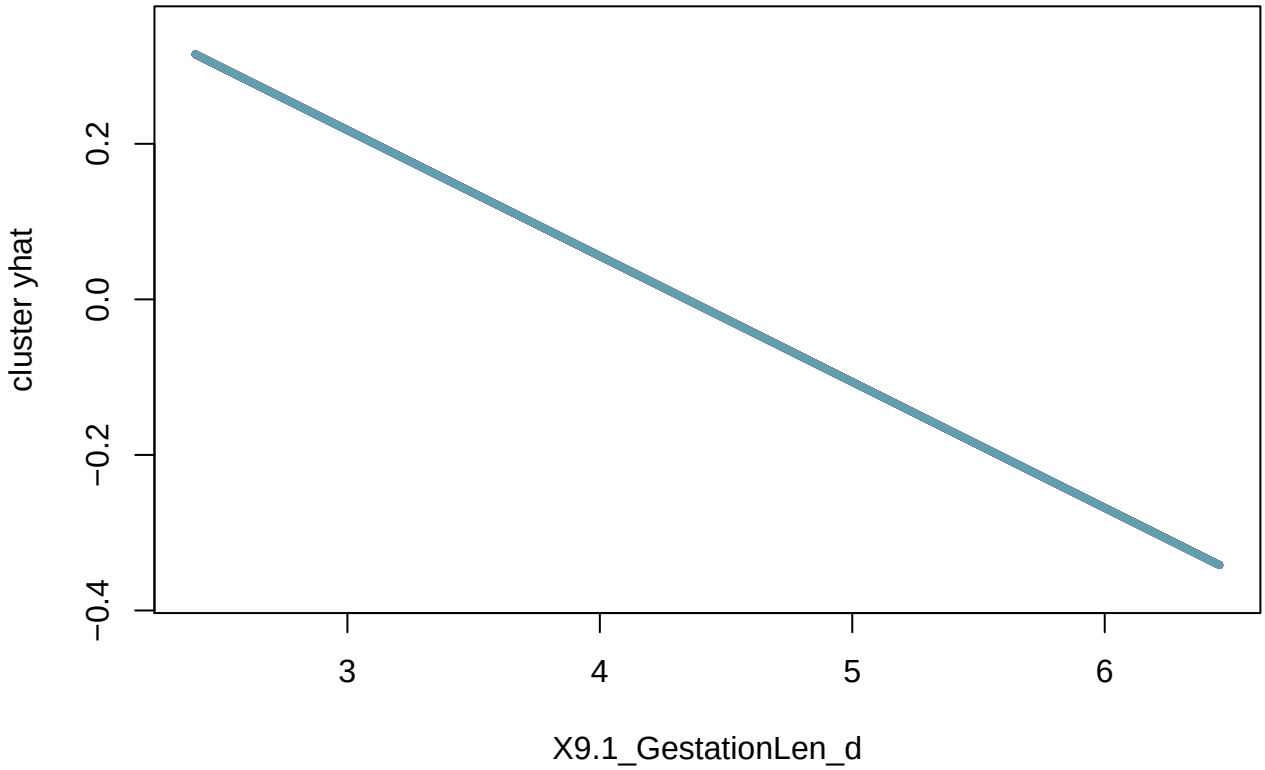
```
clusterICE(m1_enet_ice_c, nClusters = 20, centered = TRUE)
```

```
## Warning: Quick-TRANSfer stage steps exceeded maximum (= 107150)
```



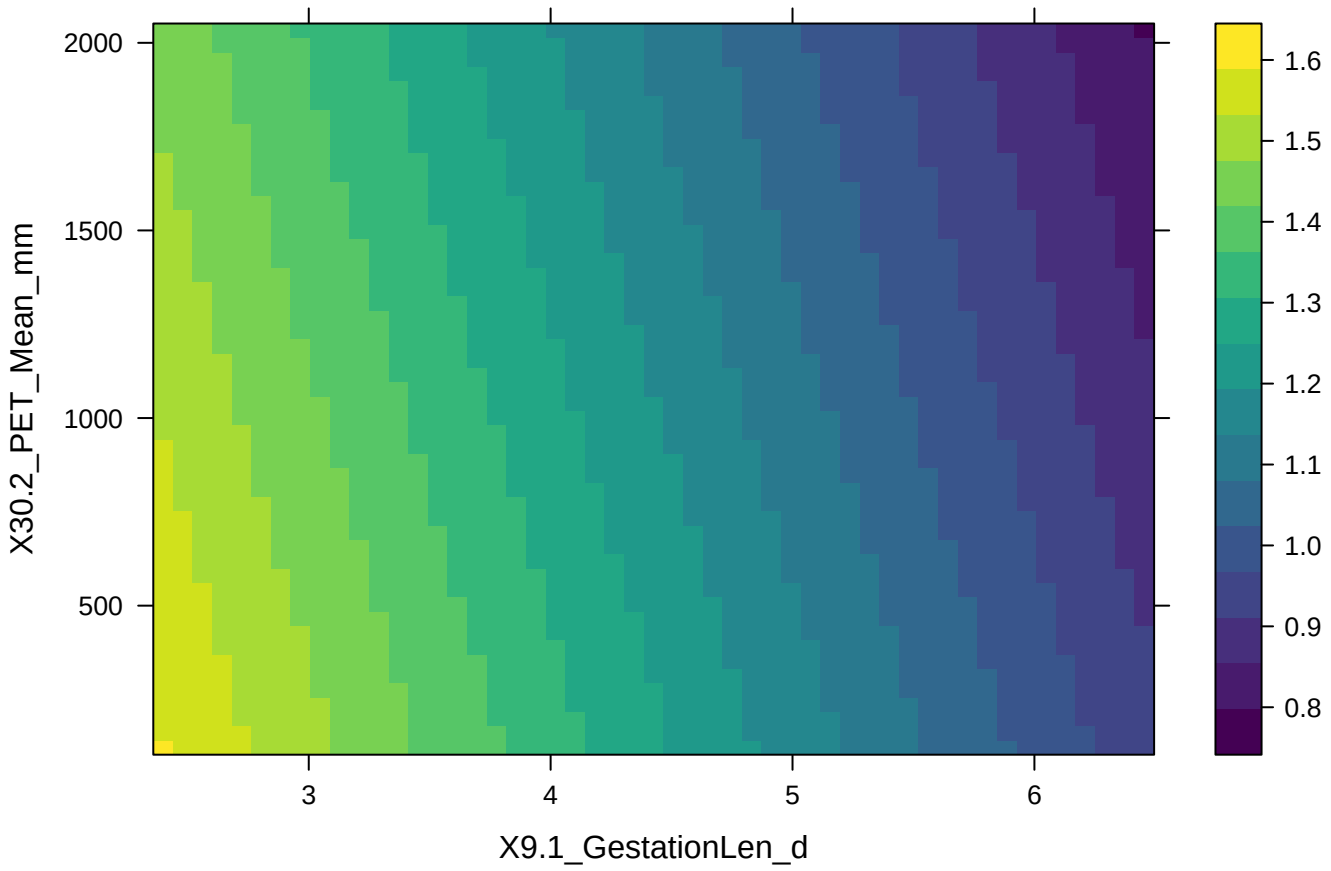

```
clusterICE(m1_enet_ice_c, nClusters = 20, centered = FALSE)
```

```
## Warning: Quick-TRANSfer stage steps exceeded maximum (= 107150)
```




```
partial(m1_enet,
        pred.var = c('X9.1_GestationLen_d', 'X30.2_PET_Mean_mm'),
        parallel = TRUE, plot = TRUE)
```

```
## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'

## Warning: <anonymous>: ... may be used in an incorrect context: '.fun(piece, ...)'
```




```
sessionInfo()
```

```
## R version 3.4.4 (2018-03-15)
## Platform: x86_64-pc-linux-gnu (64-bit)
## Running under: Ubuntu 16.04.5 LTS
##
## Matrix products: default
## BLAS: /usr/lib/libblas/libblas.so.3.6.0
## LAPACK: /usr/lib/lapack/liblapack.so.3.6.0
##
## locale:
##  [1] LC_CTYPE=en_GB.UTF-8       LC_NUMERIC=C
##  [3] LC_TIME=en_GB.UTF-8        LC_COLLATE=en_GB.UTF-8
##  [5] LC_MONETARY=en_GB.UTF-8    LC_MESSAGES=en_GB.UTF-8
##  [7] LC_PAPER=en_GB.UTF-8       LC_NAME=C
##  [9] LC_ADDRESS=C               LC_TELEPHONE=C
## [11] LC_MEASUREMENT=en_GB.UTF-8 LC_IDENTIFICATION=C
##
## attached base packages:
## [1] parallel  stats     graphics  grDevices utils     datasets  methods
## [8] base
##
## other attached packages:
##  [1] bindrcpp_0.2.2      caper_1.0.1         mvtnorm_1.0-6
##  [4] MASS_7.3-49         ape_5.2             INLA_0.0-1485844051
##  [7] Matrix_1.2-14       sp_1.3-1            elasticnet_1.1.1
## [10] lars_1.2            iml_0.7.1           ICEbox_1.1.2
## [13] sfsmisc_1.1-2       pdp_0.7.0           lime_0.4.0
## [16] caret_6.0-79        lattice_0.20-38     doParallel_1.0.10
```

```
## [19] iterators_1.0.8     foreach_1.4.3       ggplot2_3.1.0
## [22] dplyr_0.7.7         rmarkdown_1.9
##
## loaded via a namespace (and not attached):
##  [1] colorspace_1.3-2    class_7.3-14        rprojroot_1.2
##  [4] DRR_0.0.3           MatrixModels_0.4-1  prodlim_1.6.1
##  [7] lubridate_1.6.0     ranger_0.10.1       codetools_0.2-15
## [10] splines_3.4.4       mnormt_1.5-5        robustbase_0.92-8
## [13] libcoin_1.0-1       knitr_1.20.3        shinythemes_1.1.1
## [16] RcppRoll_0.2.2      Formula_1.2-2       Metrics_0.1.4
## [19] broom_0.4.2         ddalpha_1.3.2       kernlab_0.9-25
## [22] shiny_1.0.5         compiler_3.4.4      backports_1.1.0
## [25] assertthat_0.2.0    lazyeval_0.2.1      htmltools_0.3.6
## [28] tools_3.4.4         partykit_1.2-2      gtable_0.2.0
## [31] glue_1.3.0          reshape2_1.4.3      Rcpp_0.12.19
## [34] nlme_3.1-137        psych_1.7.3.21      timeDate_3043.102
## [37] inum_1.0-0          gower_0.1.2         stringr_1.3.1
## [40] mime_0.5            devtools_1.13.2     stringdist_0.9.5.1
## [43] DEoptimR_1.0-8      scales_1.0.0        ipred_0.9-6
## [46] yaml_2.1.19         memoise_1.1.0       gridExtra_2.3
## [49] rpart_4.1-13        stringi_1.2.4       randomForest_4.6-14
## [52] e1071_1.6-8         checkmate_1.8.3     lava_1.6.1
## [55] geometry_0.3-6      rlang_0.3.1         pkgconfig_2.0.2
## [58] evaluate_0.10.1     purrr_0.2.5         bindr_0.1.1
## [61] recipes_0.1.2       htmlwidgets_1.0     labeling_0.3
## [64] CVST_0.2-1          tidyselect_0.2.5    plyr_1.8.4
## [67] magrittr_1.5        R6_2.3.0            magick_2.0
## [70] dimRed_0.1.0        pillar_1.3.1        foreign_0.8-69
## [73] withr_2.1.2         mgcv_1.8-23         survival_2.43-3
## [76] abind_1.4-5         nnet_7.3-12         tibble_2.0.1
## [79] crayon_1.3.4        viridis_0.5.1       grid_3.4.4
## [82] data.table_1.12.0   ModelMetrics_1.1.0  digest_0.6.18
## [85] xtable_1.8-2        tidyr_0.8.2         httpuv_1.3.5
## [88] stats4_3.4.4        munsell_0.5.0       glmnet_2.0-16
## [91] viridisLite_0.3.0   magic_1.5-8
```

```
stopCluster(cl)
```