Statistics 360: Advanced R for Data Science

Multivariate Adaptive Regression Splines (MARS)

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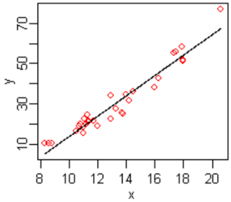
Terminology of MARS

- MARS stands for Multivariate Adaptive Regression Splines.
- Multivariate: able to generate model based on several input variables (high dimensionality).
- Adaptive: Generates flexible models in passes each time adjusting the model.
- Regression: estimation of relationship among independent and dependent variables.
- Spline: a piecewise defined polynomial function that is smooth (possesses higher order derivatives) where polynomial pieces connect.
- Knot: the point at which two polynomial pieces polynomial pieces connect.

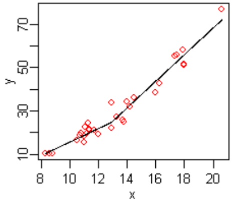
Introduction to MARS

- MARS is a form of stepwise linear regression.
- Introduced by Jerome Friedman in 1991.
- In R, this methods is implemented by package `earth`
- Suitable for higher dimensional inputs
- Extension of linear model that can model non-linearity.
- MARS models are simpler as compared to other models like random forest or neural networks.

Normal regression vs MARS



Normal Regression



MARS

$y' = -37 + 5.1x$

$y' = 25 + 6.1 \max(0, x-13) - 3.1 \max(0, 13-x)$

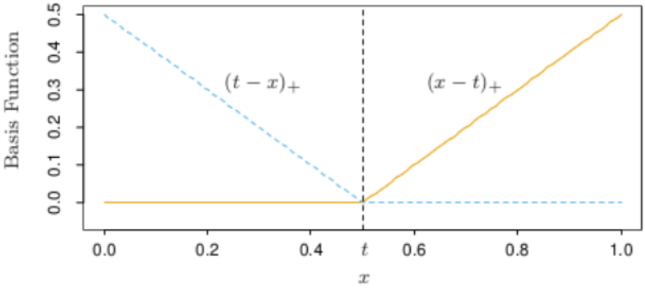
Figure 1: Linear regression vs MARS

In the MARS plot, you could see there is one knot at $x=13$.

Basis Functions

- MARS uses piecewise linear basis functions of the form $(x-t)_+$ and $(t-x)_+$. The $+$ means postive part only. so

$$(x-t)_+ = max(0, x-t), \qquad (t-x)_+ = max(0, t-x)$$



Basis Functions

- MARS uses collection of functions comprised of reflected pairs for each input x_j with knots at each observed valaue x_{ij} of that input

$$C = \{(x_j - t)_+, (t - x_j)_+\}_{t \in \{x_{1j}, x_{2j}, \dots, x_{Nj}\}, j=1,2,\dots,p.}$$

- If all input values are distinct, then set C contains 2np functions where
  - n = number of observations.
  - p = number of predictors or input variables.

MARS Model Euqation

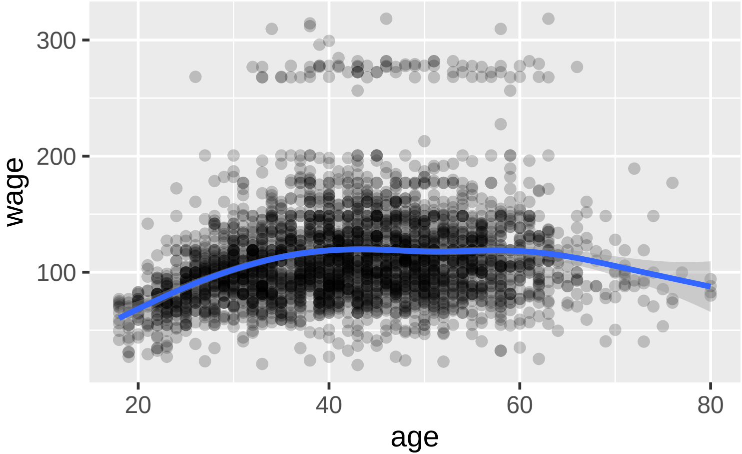
- MARS model has the general form

$$f(x) = \beta_0 + \sum_{k=1}^{M} \beta_k h_k(x)$$

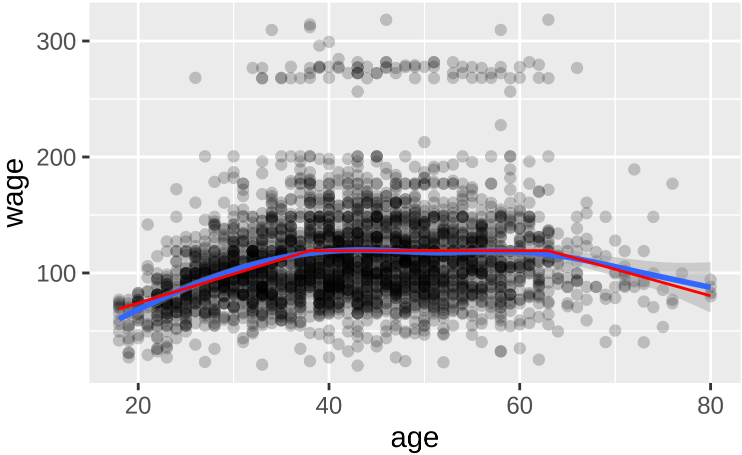
- $h_k(x)$ is a function from set C of candidate functions or a product of two or more such functions.
- βs are the coefficients estimated by minimizing the residual sum of squares (standard linear regression).
- These coefficients can be consider weights that represent the importance of the variable.

Example Data

```
library(tidyverse)
library(ISLR)
data(Wage) # help(Wage) for info
ggplot(Wage,aes(x=age,y=wage)) + geom_point(alpha=.2) + geom_smooth()
```



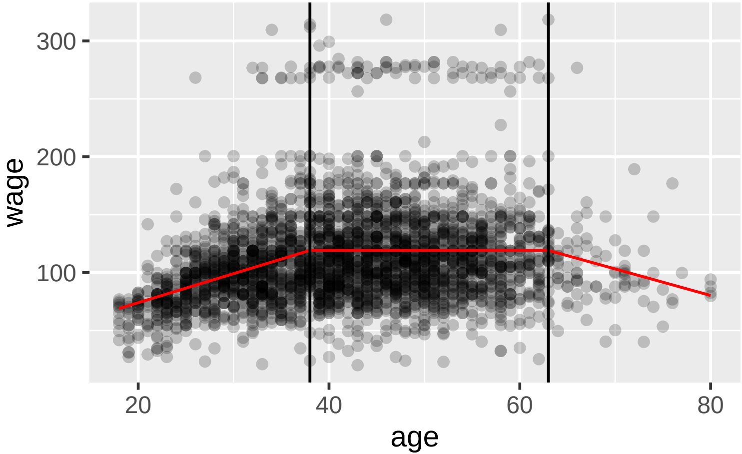
```r
library(earth)
ee <- earth(wage ~ age, data=Wage)
Wage <- mutate(Wage,pwage = predict(ee))
ggplot(Wage,aes(x=age,y=wage)) + geom_point(alpha=.2) + geom_smooth()+
  geom_line(aes(y=pwage),color="red")
```



```r
summary(ee)
```

```
## Call: earth(formula=wage~age, data=Wage)
##
##               coefficients
## (Intercept)     119.190151
## h(38-age)        -2.508377
## h(age-63)        -2.289070
##
## Selected 3 of 4 terms, and 1 of 1 predictors
## Termination condition: RSq changed by less than 0.001 at 4 terms
## Importance: age
## Number of terms at each degree of interaction: 1 2 (additive model)
## GCV 1595.44    RSS 4770379    GRSq 0.08405764    RSq 0.08649934
```

```r
ggplot(Wage,aes(x=age,y=wage)) + geom_point(alpha=.2) +
  geom_line(aes(y=pwage),color="red") +
  geom_vline(xintercept=38) +
  geom_vline(xintercept=63)
```



Hinge functions

- The points 38 and 63 are "knots" where the piece-wise linear function changes slope.
- The piece-wise linear fit is a linear model in a constant term (intercept) and two "hinge" functions, $h(38 - age)$ and $h(age - 63)$, where

$$h(x) = \max(0, x)$$

- Hinge functions $h(x - c)$ and $h(c - x)$ are called mirror image.
  - Exercise: Plot two mirror-image hinge functions for `x <- seq(from=0,to=50,length=100)` and `c<-50`. Why are they called mirror image?

Fitting

- Once we are given the knots and hinge functions, the fit can be obtained by least squares.

```
Wage <- mutate(Wage,h1=pmax(0,38-age),h2=pmax(0,age-63))
ff <- lm(wage ~ h1+h2,data=Wage)
summary(ff)$coefficients
```

```
##               Estimate Std. Error    t value     Pr(>|t|)
## (Intercept) 119.190151  0.8539353 139.577500 0.000000e+00
## h1           -2.508377  0.1506008 -16.655805 1.216314e-59
## h2           -2.289070  0.5949343  -3.847601 1.217668e-04
```

Simulation study - Generating data

```r
set.seed(360)
x <- seq(1,10,by=1)
h5x <- pmax(0,5-x);
hx5 <- pmax(0,x-5)
#plot(x,h5x,type="l",col="blue",lty=2,xlab="x",ylim=c(0,10))
#lines(x,hx5, lty=2,col="red")
y <- 1+2*h5x+3*hx5+rnorm(10,0,1);
cbind(x,h5x,hx5,y)
```

```
##        x h5x hx5          y
##  [1,]  1   4   0 10.4374946
##  [2,]  2   3   0  7.3225732
##  [3,]  3   2   0  4.7957034
##  [4,]  4   1   0  2.0009050
##  [5,]  5   0   0  0.9624999
##  [6,]  6   0   1  3.2485689
##  [7,]  7   0   2  6.3494051
##  [8,]  8   0   3  9.8481529
##  [9,]  9   0   4 12.1619673
## [10,] 10   0   5 16.5373044
```

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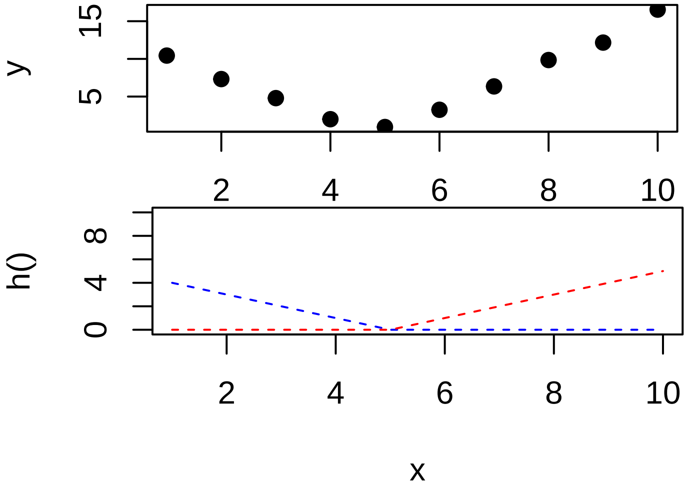
y
5
15
2
4
6
8
10
h()
0
4
8
2
4
6
8
10
x

Simulation study: fitted coefficients with earth

```r
mod <- earth(y ~ x);
summary(mod)
```

```
## Call: earth(formula=y~x)
##
##             coefficients
## (Intercept)    0.1304094
## h(5-x)         2.4668639
## h(x-5)         3.1794562
##
## Selected 3 of 3 terms, and 1 of 1 predictors
## Termination condition: RSq changed by less than 0.001 at 3 terms
## Importance: x
## Number of terms at each degree of interaction: 1 2 (additive model)
## GCV 0.8571923    RSS 2.142981    GRSq 0.9680172    RSq 0.9901288
```

Simulation study: fitted coefficients with `lm()`

```
mod2 <- lm(y~h5x+hx5);
summary(mod2)
```

```
##
## Call:
## lm(formula = y ~ h5x + hx5)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -0.6863 -0.2534 -0.1006  0.3746  0.8321
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   0.1304     0.3448   0.378    0.716
## h5x           2.4669     0.1530  16.123 8.59e-07 ***
## hx5           3.1795     0.1200  26.489 2.80e-08 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.5533 on 7 degrees of freedom
## Multiple R-squared:  0.9901, Adjusted R-squared:  0.9873
## F-statistic: 351.1 on 2 and 7 DF,  p-value: 9.557e-08
```

Questions

For a given dataset

- How do we choose the knots?
- What happens when there are multiple explanatory variables, and we allow for interactions between them?

MARS Model Building Procedure

1. Gather data: x input variables with y observations each, giving a total of xy data points.
2. Calculate set of candidate functions by generating reflected pairs of basis functions with knows set at observed values.
3. Specify constraints; the number of terms in the model and maxium allowable degree of interaction.
4. Do foward pass: try out new fucntion products and see which product decreases training error.
5. Do backward pass: fix overfit.
6. Do generalized cross validation to estimate the optimal number of terms in the model.

MARS Forward Pass

- At each step, MARS adds the basis function which reduces the residual error the most
- Always adds the basis function in "pairs", both sides of knot
- Calculate value for knot and function that fit the data, least squares.
- This is greedy algorithm.
- The addition of model terms continues until the max number of terms in the model is reached.

MARS Backwards Pass

- Remove one term at a time from the model
- Remove the term which increases the residual error the least
- Continue removing terms until cross validation is statisfied
- Use the Generalized Cross Validation (GCV) function for this purpose.

Reference

1. Hastie, Tibshirani, and Friedman. The Elements of Statistical Learning (2nd ed.). Springer, 2009. http://www-stat.stanford.edu/~hastie/pub.htm.
2. Jerome H. Friedman. Multivariate Adaptive Regression Splines (with discussion). Annals of Statistics, 1991