GENERALIZED ADDITIVE MODELS

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GENERAL STRUCTURE

Generalized Additive Models (GAMs)

- Provides **general** framework for **adding** of non-linear functions together instead of the typical linear structure.

$$y = \beta_0 + f_1(x_1) + f_2(x_2) + \cdots + f_p(x_p) + \varepsilon$$

- Can be used for regression or classification problems.

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Adding **potentially** complex, individual relationships together.

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- Can be used for regression or classification problems.

Many potential complex relationships to try and model with.

PIECEWISE LINEAR REGRESSION

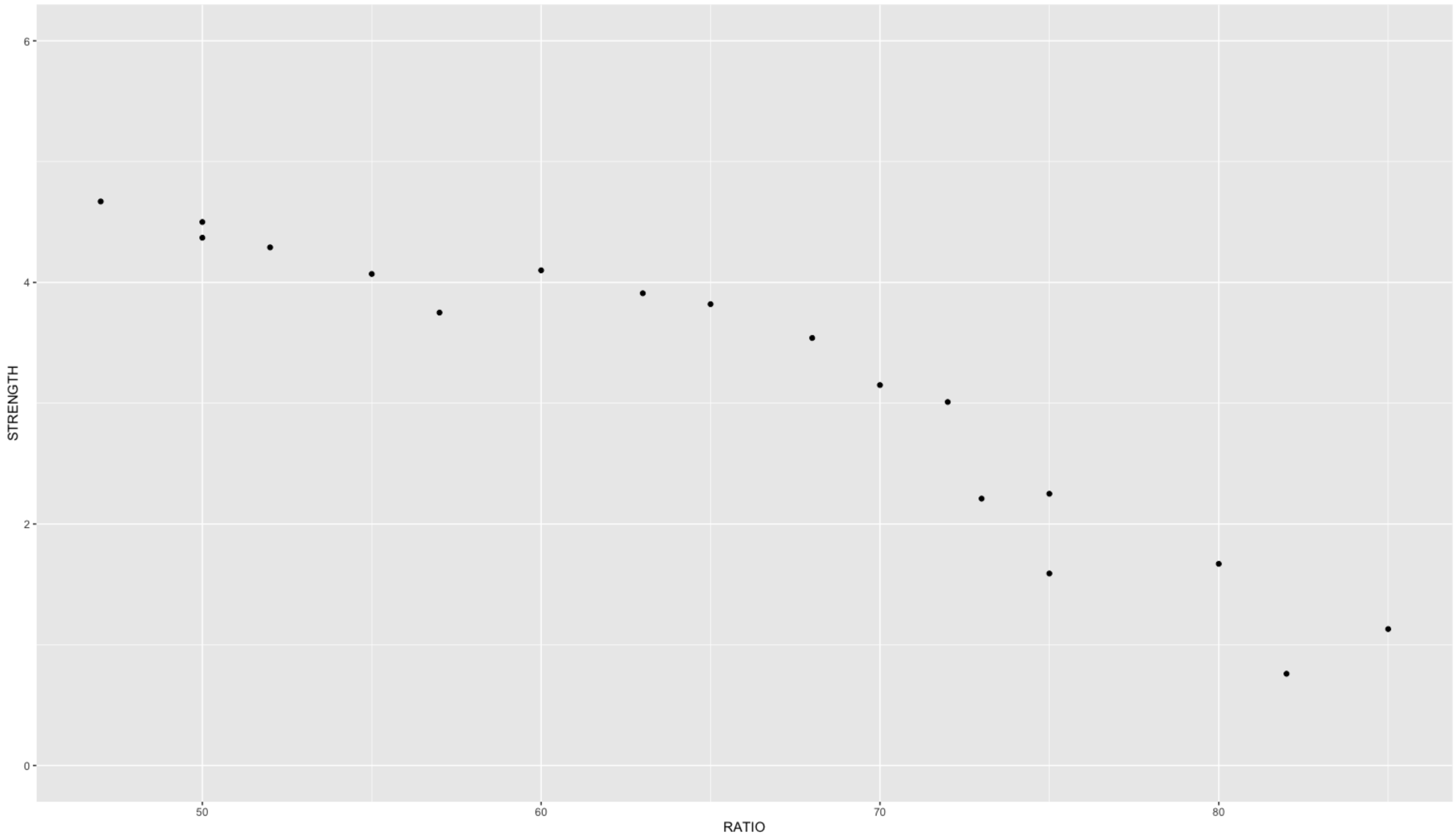
Changing Slopes

- The slope of the linear relationship between a predictor variable and a response variable can change over different values of the predictor variable.
- Typical straight-line model $\hat{y} = \beta_0 + \beta_1 x_1$ will not be a good fit for this type of data.

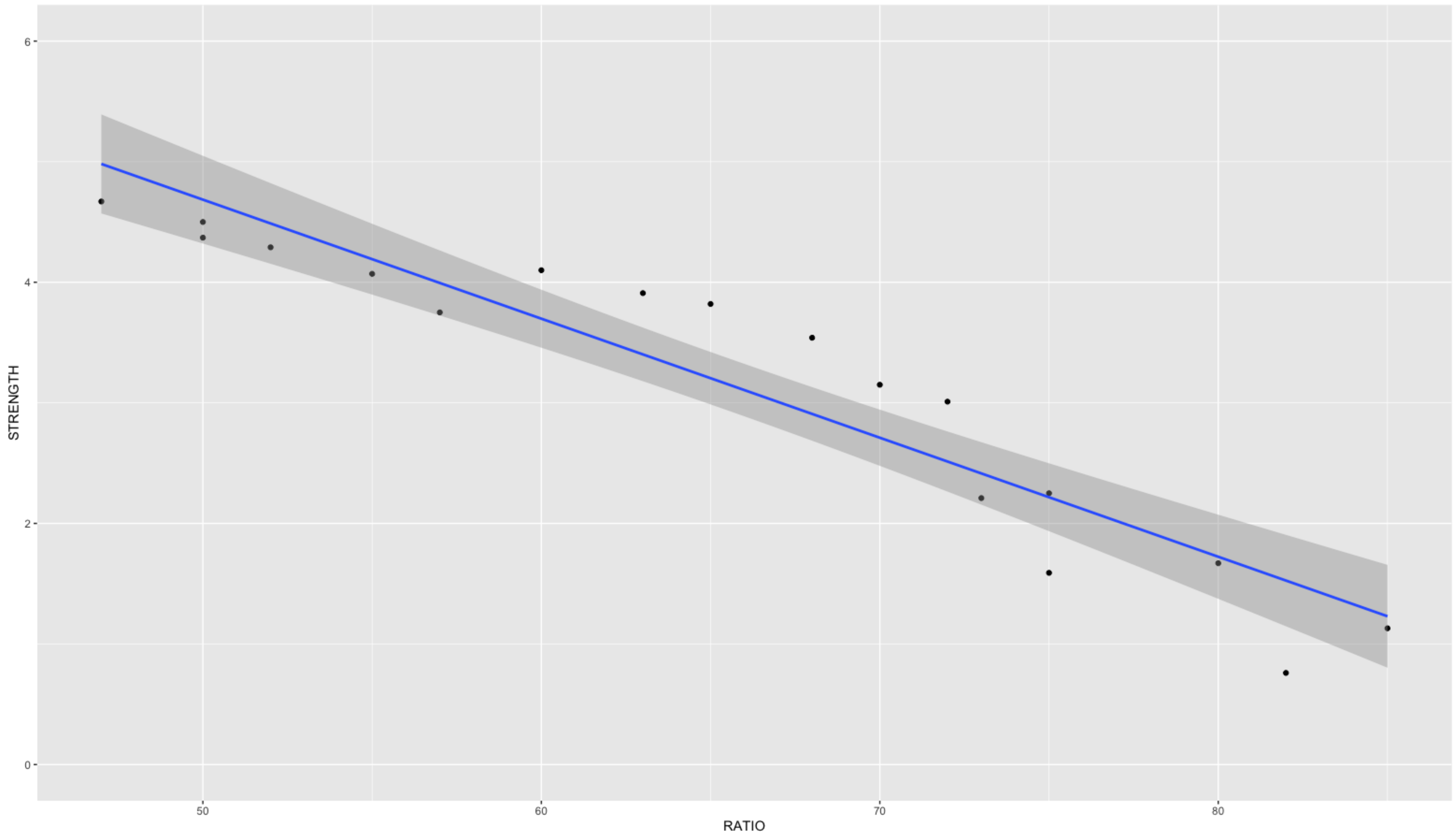
Cement Data

- The comprehensive strength of concrete depends on the proportion of water mixed with cement.
- The comprehensive strength decreases at a much faster rate for batches with a greater than 70% water/cement ratio.

Changing Slopes



Changing Slopes



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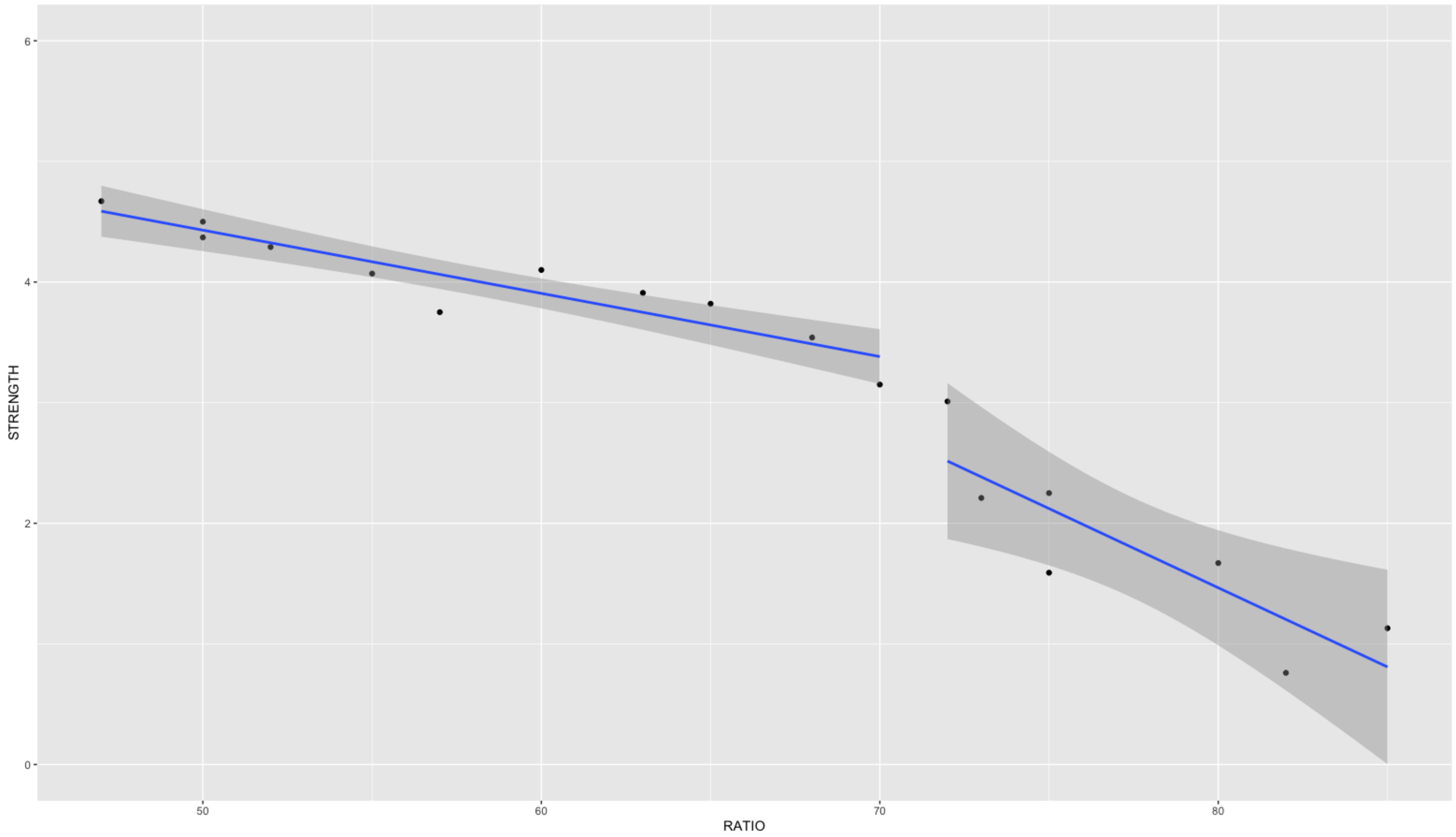

Piecewise Linear Regression

- A model where different straight-line relationships for different intervals in the predictor variable is called the **piecewise linear regression model**.
- The model is the following for two slopes:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 (x_1 - k) x_2 + \varepsilon$$

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Knot value for x_1.

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$$y = \beta_0 + \beta_1 x_1 + \varepsilon$$

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$$y = \beta_0 + \beta_1 x_1 + \beta_2 (x_1 - k) x_2 + \varepsilon$$

$x_2 = 0$

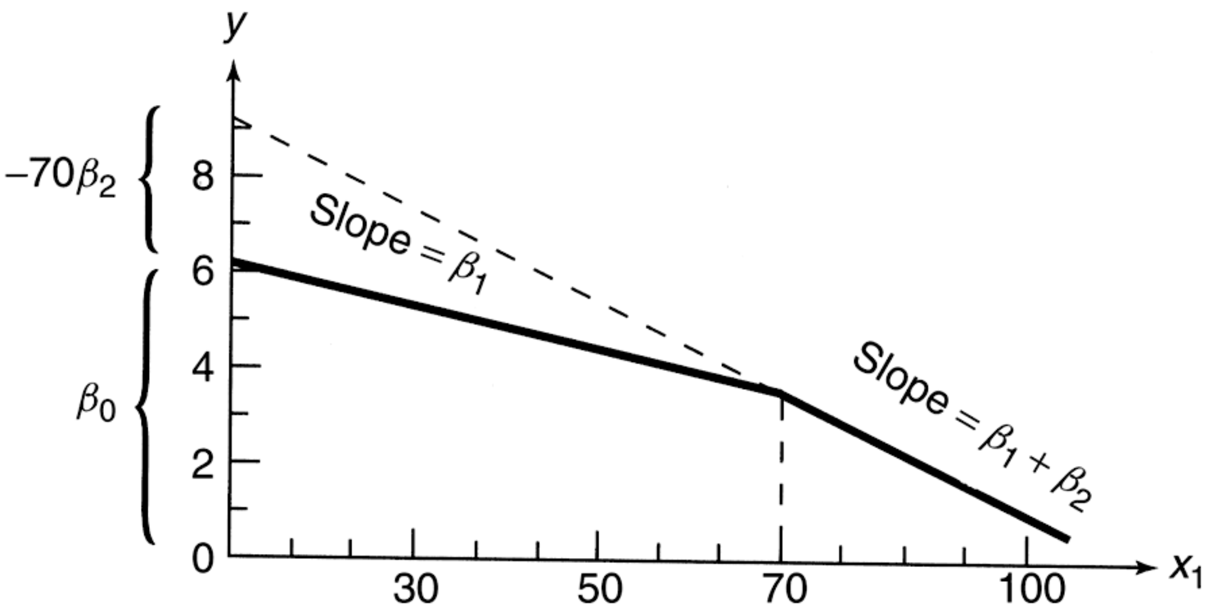
$$y = \beta_0 + \beta_1 x_1 + \varepsilon$$

$x_2 = 1$

$$y = (\beta_0 - k\beta_2) + (\beta_1 + \beta_2) x_1 + \varepsilon$$

Cement Data

- The comprehensive strength of concrete depends on the proportion of water mixed with cement.
- The comprehensive strength decreases at a much faster rate for batches with a greater than 70% water/cement ratio.



Piecewise Linear Regression

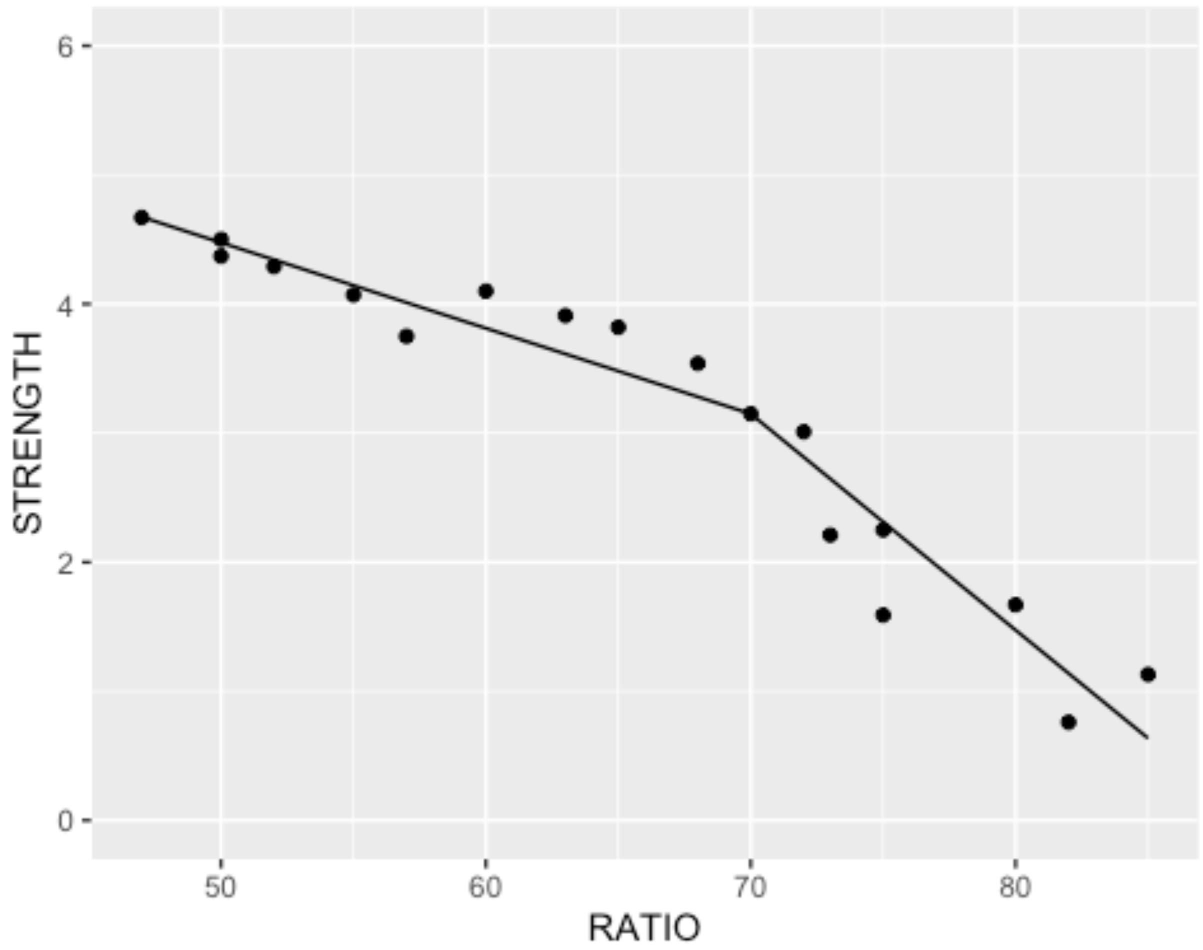
```
cement.lm <- lm(STRENGTH ~ RATIO + X2STAR, data = cement)

summary(cement.lm)
```

$(x_1 - k)x_2$

```
## Call:
## lm(formula = STRENGTH ~ RATIO + X2STAR, data = cement)
##
## Residuals:
##       Min        1Q    Median        3Q       Max
## -0.72124 -0.09753 -0.00163  0.24297  0.49393
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  7.79198    0.67696  11.510 7.62e-09 ***
## RATIO       -0.06633    0.01123  -5.904 2.89e-05 ***
## X2STAR      -0.10119    0.02812  -3.598  0.00264 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.3286 on 15 degrees of freedom
## Multiple R-squared:  0.9385, Adjusted R-squared:  0.9303
## F-statistic: 114.4 on 2 and 15 DF,  p-value: 8.257e-10
```

Piecewise Linear Regression

```
ggplot(cement, aes(x = RATIO, y = STRENGTH)) +
  geom_point() +
  geom_line(data = cement, aes(x = RATIO,
            y = cement.lm$fitted.values)) +
  ylim(0,6)
```



Extensions – Discontinuous

- The previous approach dealt with piecewise functions that are continuous.
- The following is the discontinuous set-up for two straight lines:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 (x_1 - k) x_2 + \beta_3 x_2 + \varepsilon$$

$$x_2 = \begin{cases} 1, & x_1 > k \\ 0, & x_1 \leq k \end{cases}$$

Extensions – Discontinuous

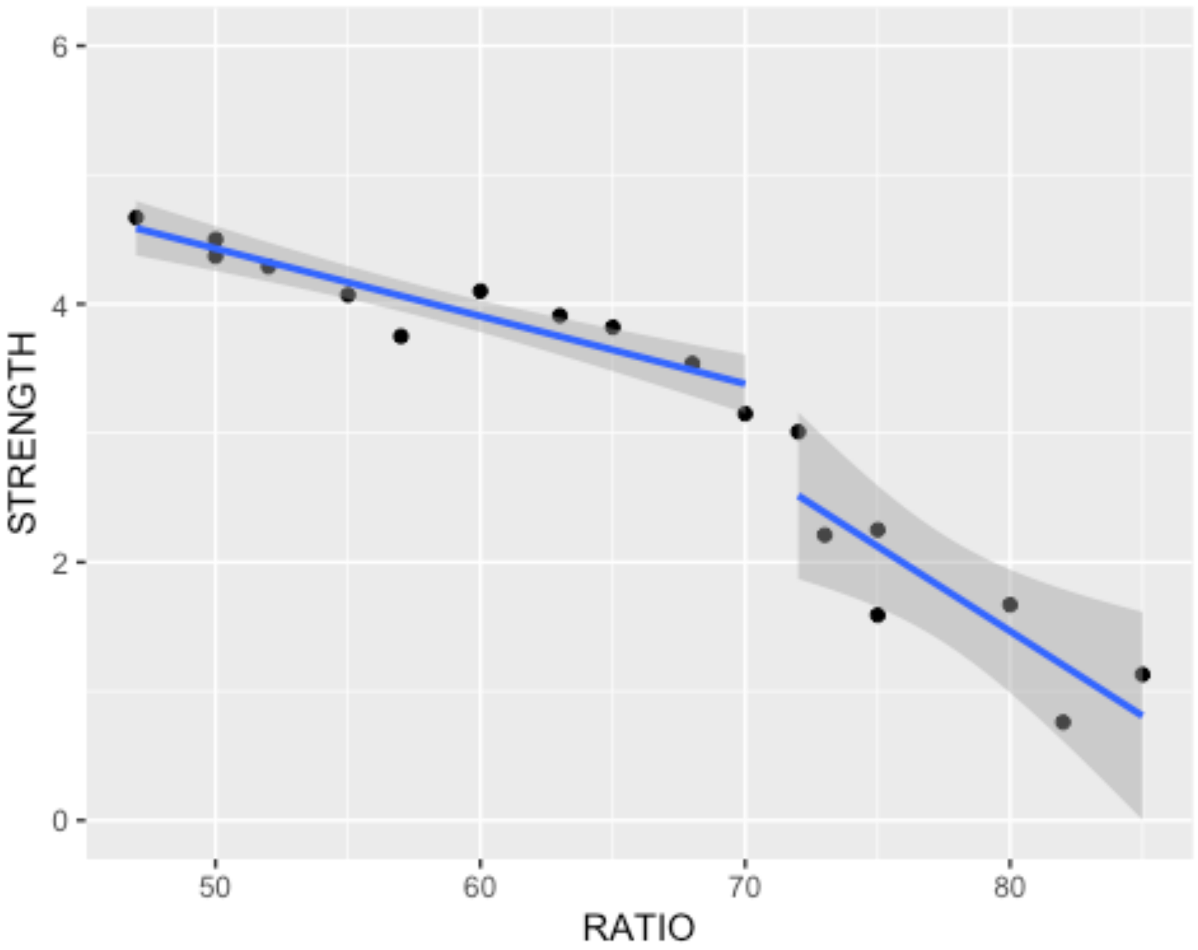
```
cement.lm <- lm(STRENGTH ~ RATIO + X2STAR + X2, data = cement)

summary(cement.lm)
```

$(x_1 - k)x_2$

```
##
## Call:
## lm(formula = STRENGTH ~ RATIO + X2STAR + X2, data = cement)
##
## Residuals:
##       Min       1Q   Median       3Q      Max
## -0.53167 -0.15513  0.06171  0.17239  0.49451
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept)  7.04975    0.68558  10.283  6.6e-08 ***
## RATIO       -0.05240    0.01174  -4.463 0.000536 ***
## X2STAR      -0.07888    0.02686  -2.937 0.010830 *
## X2          -0.60388    0.26877  -2.247 0.041302 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.2916 on 14 degrees of freedom
## Multiple R-squared:  0.9548, Adjusted R-squared:  0.9451
## F-statistic: 98.57 on 3 and 14 DF,  p-value: 1.188e-09
```

Extensions – Discontinuous

```
qplot(RATIO, STRENGTH, group = X2,
      geom = c('point', 'smooth’),
      method = 'lm', data = cement,
      ylim = c(0,6))
```



Extensions

- The same modeling approach can be applied to any piecewise regression.
- The following is the set-up for three straight lines:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 (x_1 - k_1) x_2 + \beta_3 (x_1 - k_2) x_3 + \varepsilon$$

$$x_2 = \begin{cases} 1, & x_1 > k_1 \\ 0, & \text{if not} \end{cases} \qquad x_3 = \begin{cases} 1, & x_1 > k_2 \\ 0, & \text{if not} \end{cases}$$

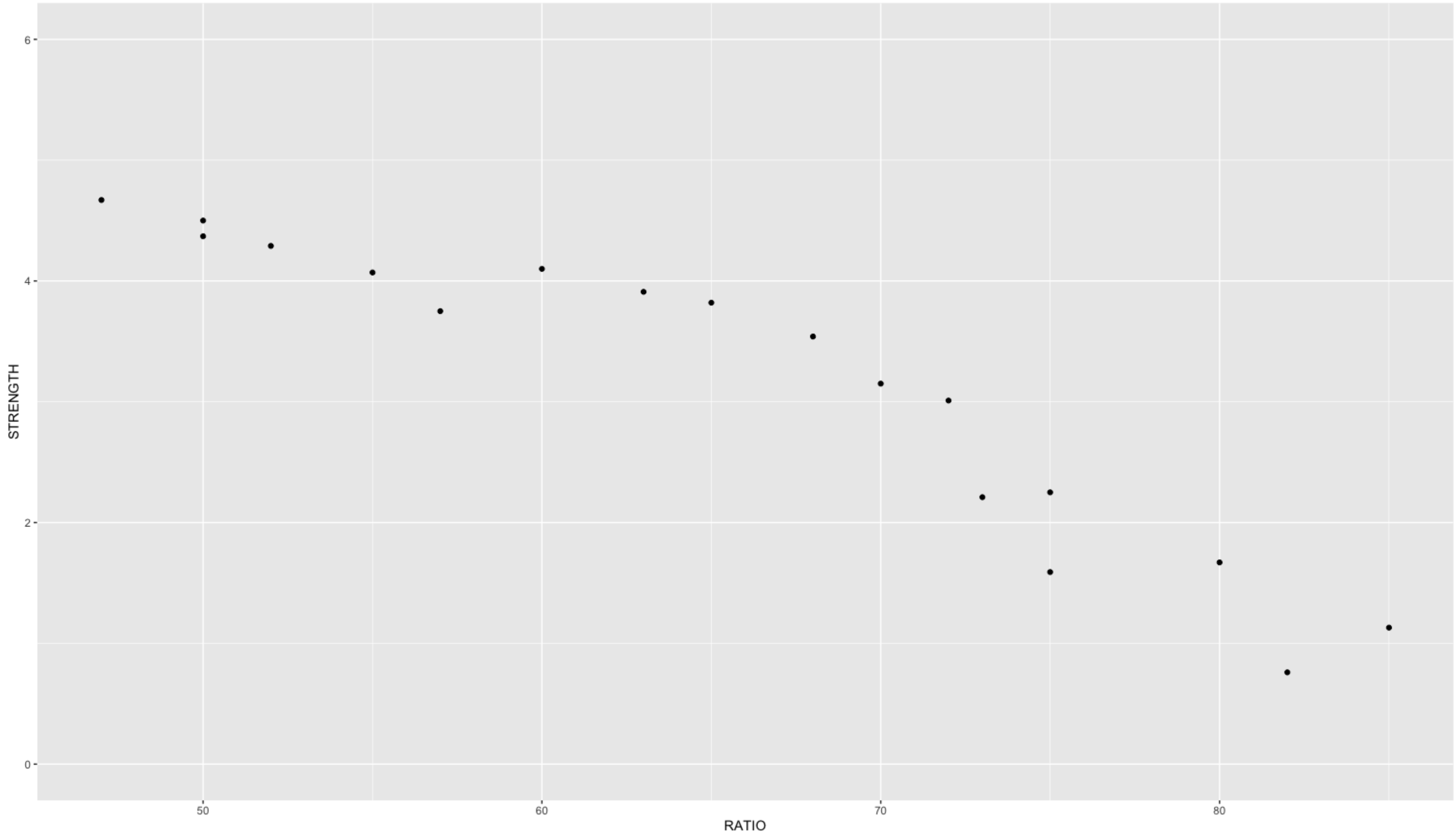
MARS (AND EARTH)

Multivariate Adaptive Regression Splines (MARS)

- Multivariate adaptive regression splines (MARS) is a non-parametric technique that is still has a linear form to the model (additive) but has nonlinearities and interaction between variables.
- Essentially, uses **piecewise** regression approach to split into pieces then potentially uses either linear or nonlinear patterns for each piece.

Knots

- MARS first looks for the point in the range of *x* where two linear functions on either side of the point provides the least squared error (linear regression).



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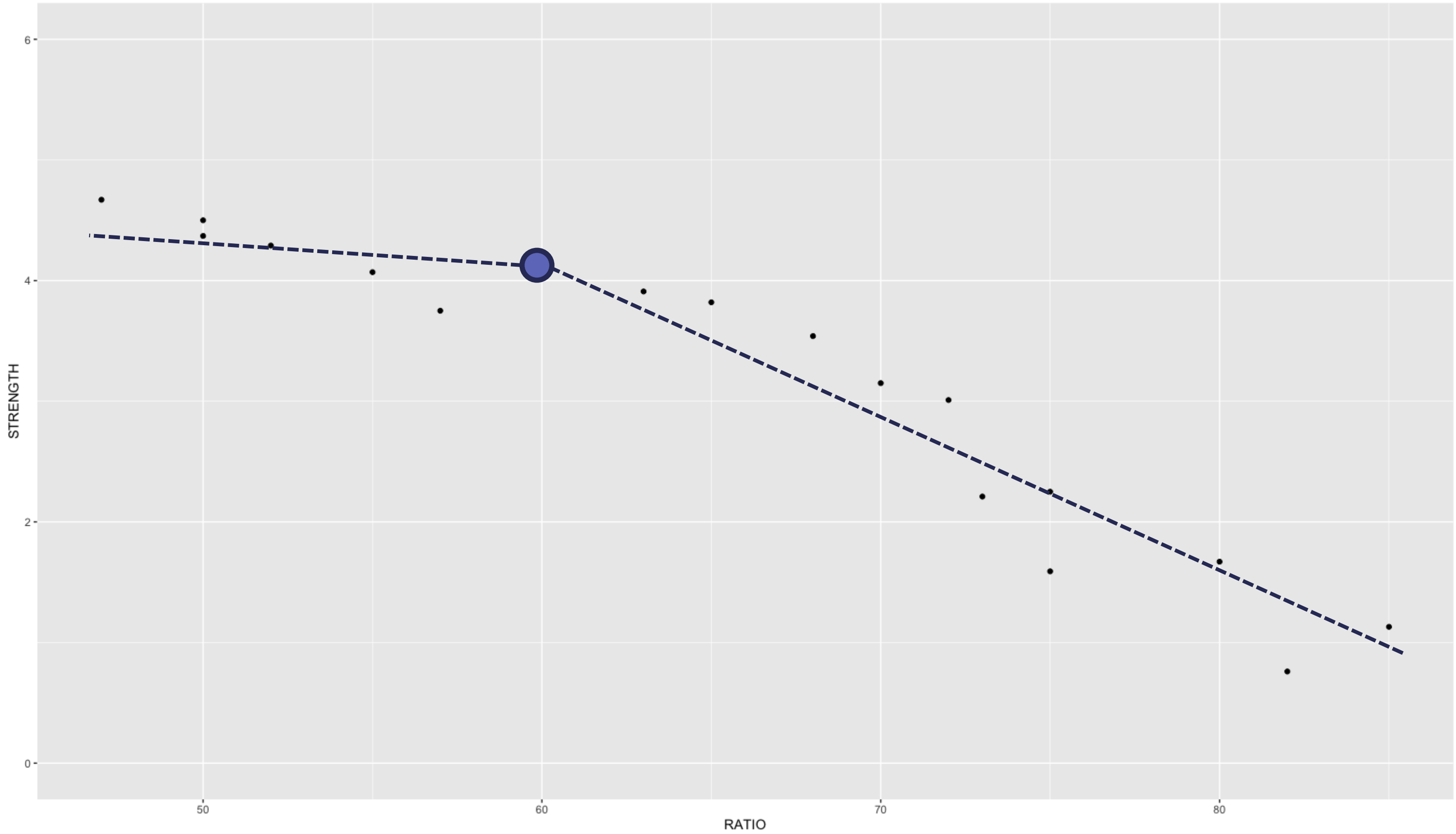

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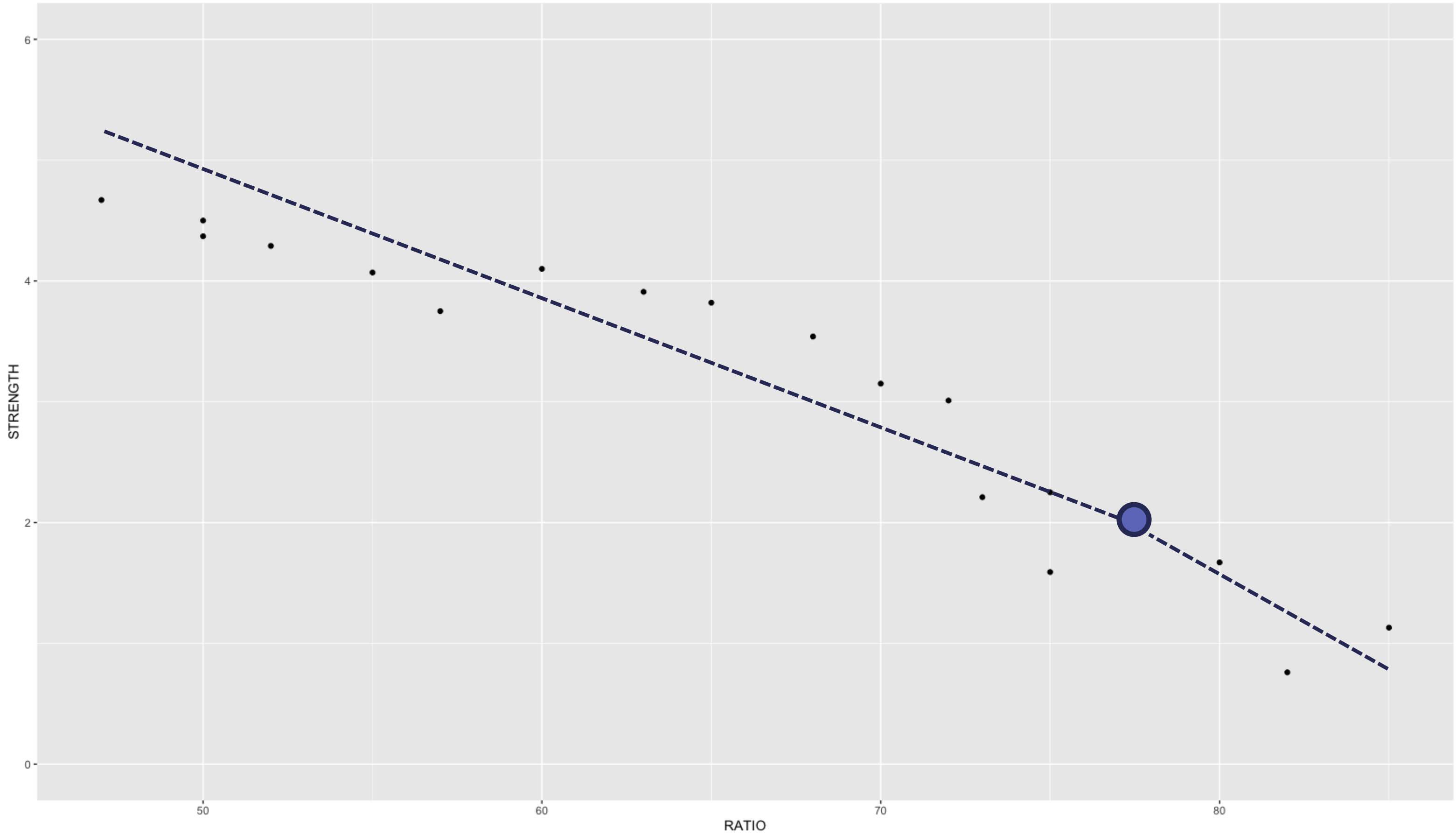

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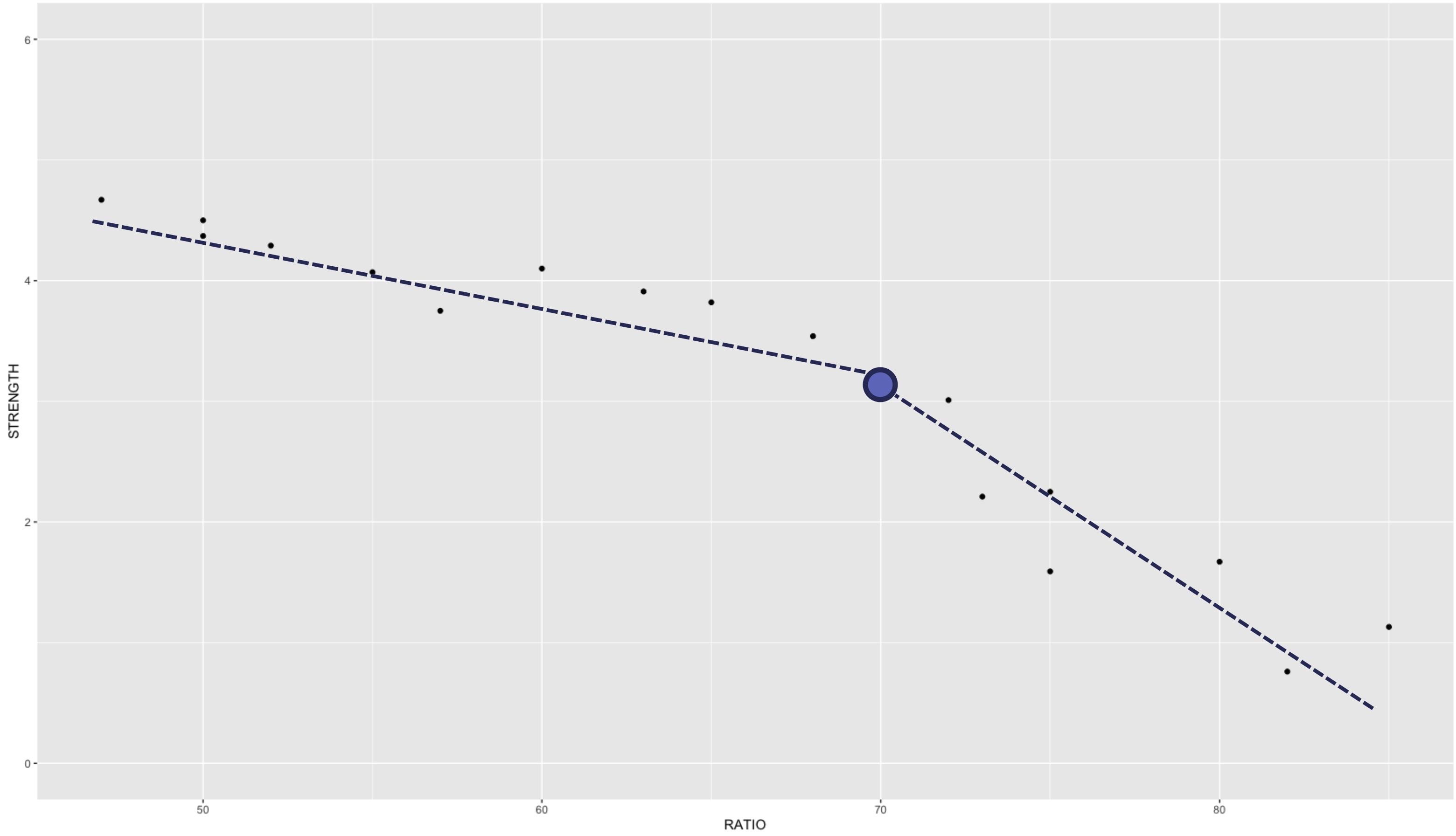
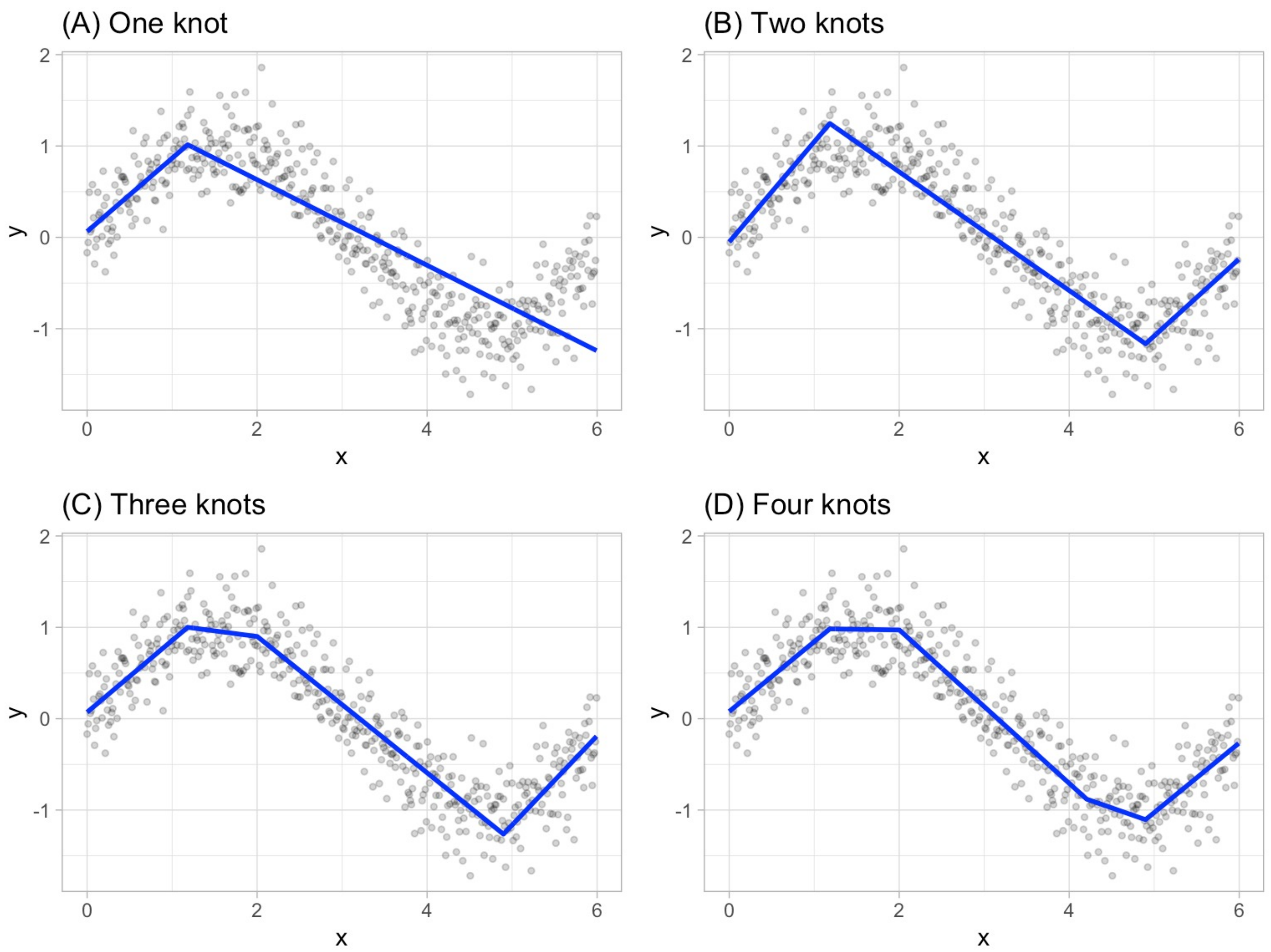


Many Knots



How Many Knots?

- Algorithm continues on each piece of the piecewise function until many knots are found (WILL OVERFIT YOUR DATA).
- Then works backwards (“prunes”) to remove knots that do not contribute significantly to out of sample accuracy.
  - Calculation is performed by the generalized cross-validation (GCV) procedure – computational shortcut for leave-one-out cross-validation.

- **Does this for all variables!**

$$y = \beta_0 + f_1(x_1) + f_2(x_2) + \cdots + f_p(x_p) + \varepsilon$$

EARTH

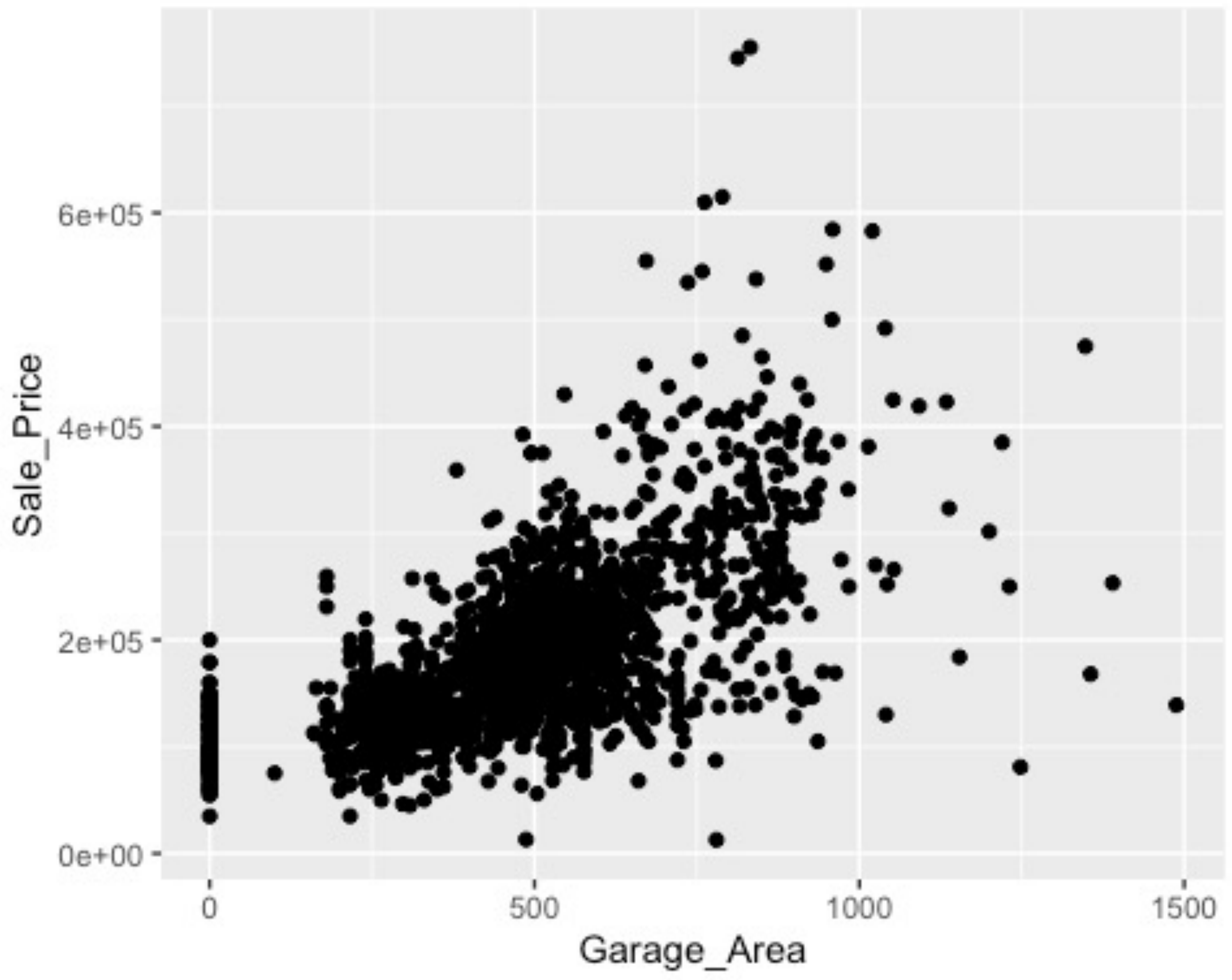
- **E**nhanced **A**daptive **R**egression **T**hrough **H**inges (EARTH) is the implementation of the MARS algorithm in most software.
- MARS is trademarked by Salford Systems, so instead we use EARTH.

EARTH (and MARS)

```r
ames <- make_ordinal_ames()

ames <- ames %>% mutate(id = row_number())

set.seed(4321)

training <- ames %>% sample_frac(0.7)
testing <- anti_join(ames, training, by = 'id')

training <- training %>%
  select(Sale_Price, Bedroom_AbvGr, Year_Built, Mo_Sold, Lot_Area, Street,
         Central_Air, First_Flr_SF, Second_Flr_SF, Full_Bath, Half_Bath, Fireplaces,
         Garage_Area, Gr_Liv_Area, TotRms_AbvGrd)
```

EARTH (and MARS)

```
ggplot(training, aes(x = Garage_Area,
                     y = Sale_Price)) +
  geom_point()
```



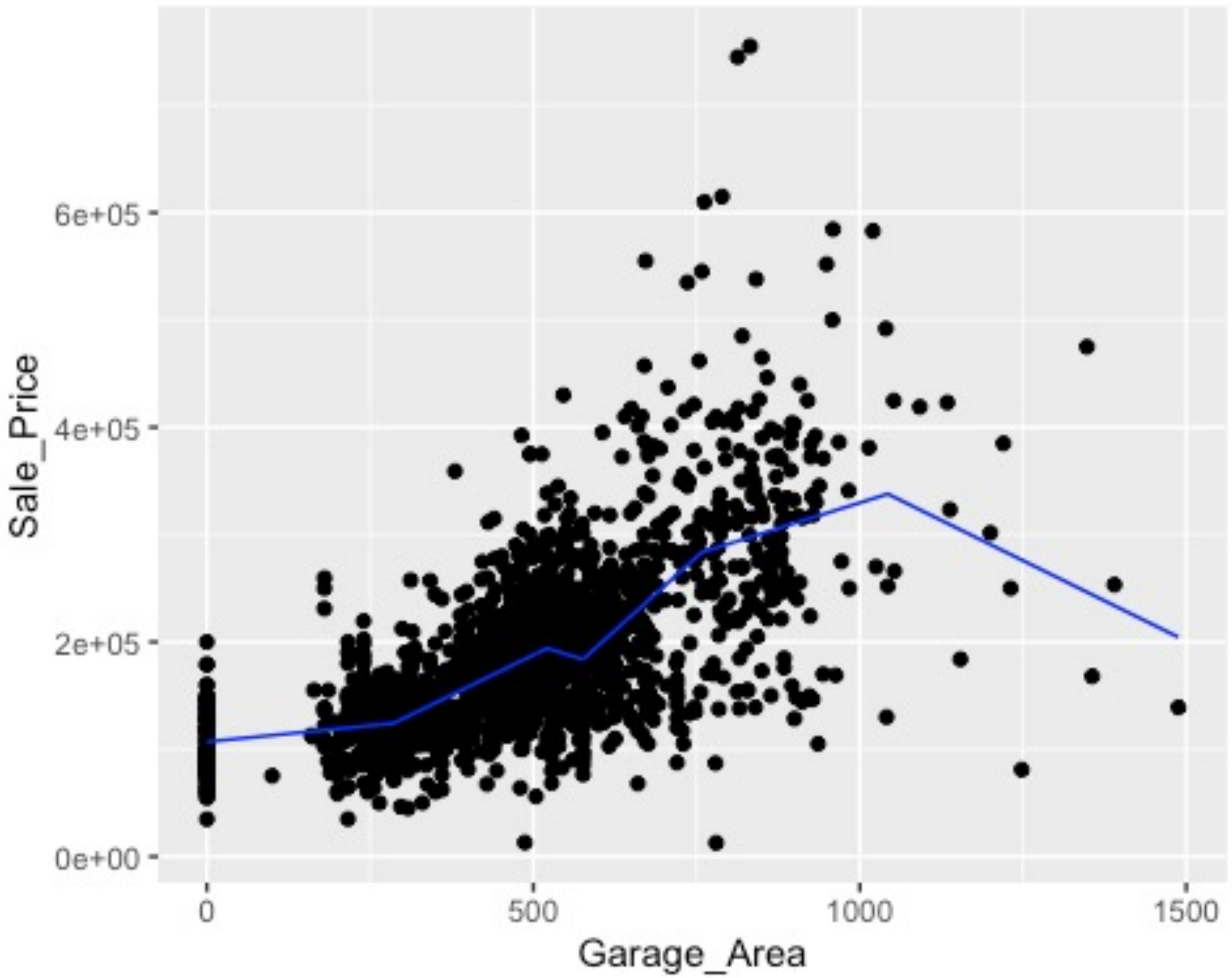
EARTH (and MARS)

```
mars1 <- earth(Sale_Price ~ Garage_Area, data = training)
summary(mars1)
```

```
## Call: earth(formula=Sale_Price~Garage_Area, data=training)
##
##                        coefficients
## (Intercept)              124159.039
## h(286-Garage_Area)          -60.257
## h(Garage_Area-286)          297.277
## h(Garage_Area-521)         -483.642
## h(Garage_Area-576)          733.859
## h(Garage_Area-758)         -356.460
## h(Garage_Area-1043)        -490.873
##
## Selected 7 of 7 terms, and 1 of 1 predictors
## Termination condition: RSq changed by less than 0.001 at 7 terms
## Importance: Garage_Area
## Number of terms at each degree of interaction: 1 6 (additive model)
## GCV 3427475346    RSS 6.94092e+12    GRSq 0.4492014    RSq 0.4556309
```

EARTH (and MARS)

```
ggplot(training, aes(x = Garage_Area,
                     y = Sale_Price)) +
  geom_point() +
  geom_line(data = training,
            aes(x = Garage_Area,
                y = mars1$fitted.values),
            color = "blue")
```



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mars1 <- earth(Sale_Price ~ ., data = training)
summary(mars1)
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```
## Call: earth(formula=Sale_Price~., data=training)
##
##                           coefficients
## (Intercept)                  319493.46
## Central_AirY                  20289.49
## h(4-Bedroom_AbvGr)             9214.66
## h(Bedroom_AbvGr-4)           -23009.05
...
## h(Half_Bath-1)               -45378.31
## h(2-Fireplaces)              -14408.56
## h(Fireplaces-2)              -26072.58
## h(Garage_Area-539)              101.97
## h(Garage_Area-1043)            -294.30
## h(Gr_Liv_Area-2049)              65.21
## h(Gr_Liv_Area-3194)            -159.79
##
## Selected 21 of 24 terms, and 10 of 14 predictors
## Termination condition: Reached nk 29
## Importance: First_Flr_SF, Second_Flr_SF, Year_Built, Garage_Area, ...
## Number of terms at each degree of interaction: 1 20 (additive model)
## GCV 1033819964    RSS 2.036439e+12    GRSq 0.8338641    RSq 0.8402842
```

Variable Importance

```
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##                          coefficients
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```

Variable Importance

- There is one “subset” for each model size (1 term, 2 terms, etc.) – the best model of that size.
- Ranks variables by how many of the subsets that variable appears in.
  - More subsets of models it appears in (in the best 1 variable model, in the best 2 variable model, etc.), then the better the variable.
- RSS (residual sum of squares or sum of squares error) is scaled version of decrease in residual sum of squares relative to the previous subset.
- GCV is approximation of RSS on leave-one-out-cross validation.

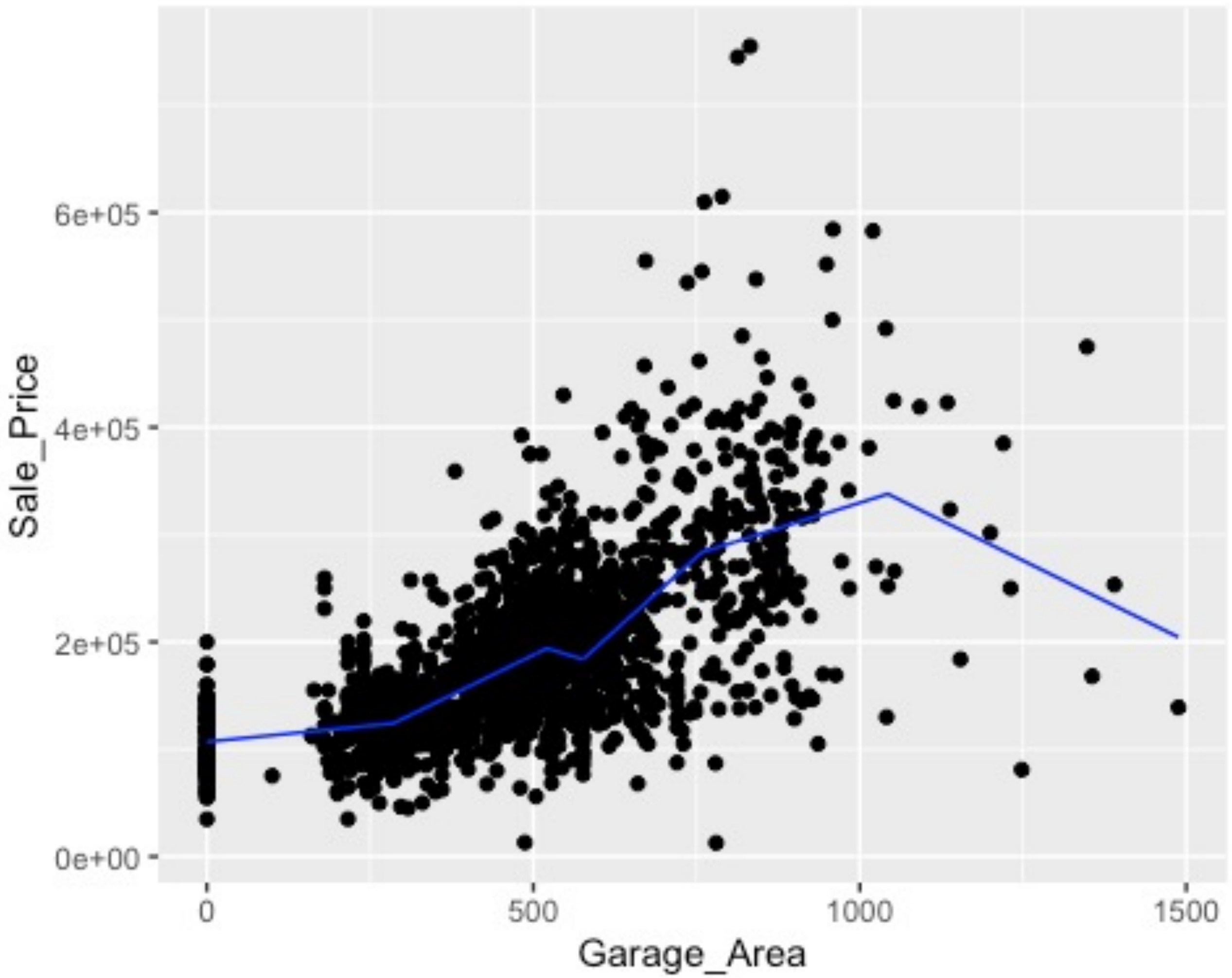
Variable Importance

```
evimp(mars1)
```

```
##                  nsubsets   gcv    rss
## First_Flr_SF           20 100.0  100.0
## Second_Flr_SF          19  71.7   71.9
## Year_Built             18  50.9   51.3
## Garage_Area            17  34.3   35.0
## Fireplaces             16  31.0   31.7
## Gr_Liv_Area            15  27.6   28.4
## Central_AirY           12  20.0   20.9
## Bedroom_AbvGr          11  18.1   19.0
## Lot_Area               10  16.2   17.2
## Half_Bath               4   7.4    8.2
```

Interpretability

- Can view the “relationship” between predictors and target variable.



SMOOTHING

Smoothing

- GAMs can be made up of any non-parametric function of the predictor variables.
- Another popular technique is to use **smoothing functions** so the piecewise linear regressions are not so jagged.
- Many different types of smoothing functions:
  - LOESS (localized regression)
  - Smoothing splines
  - Regression splines

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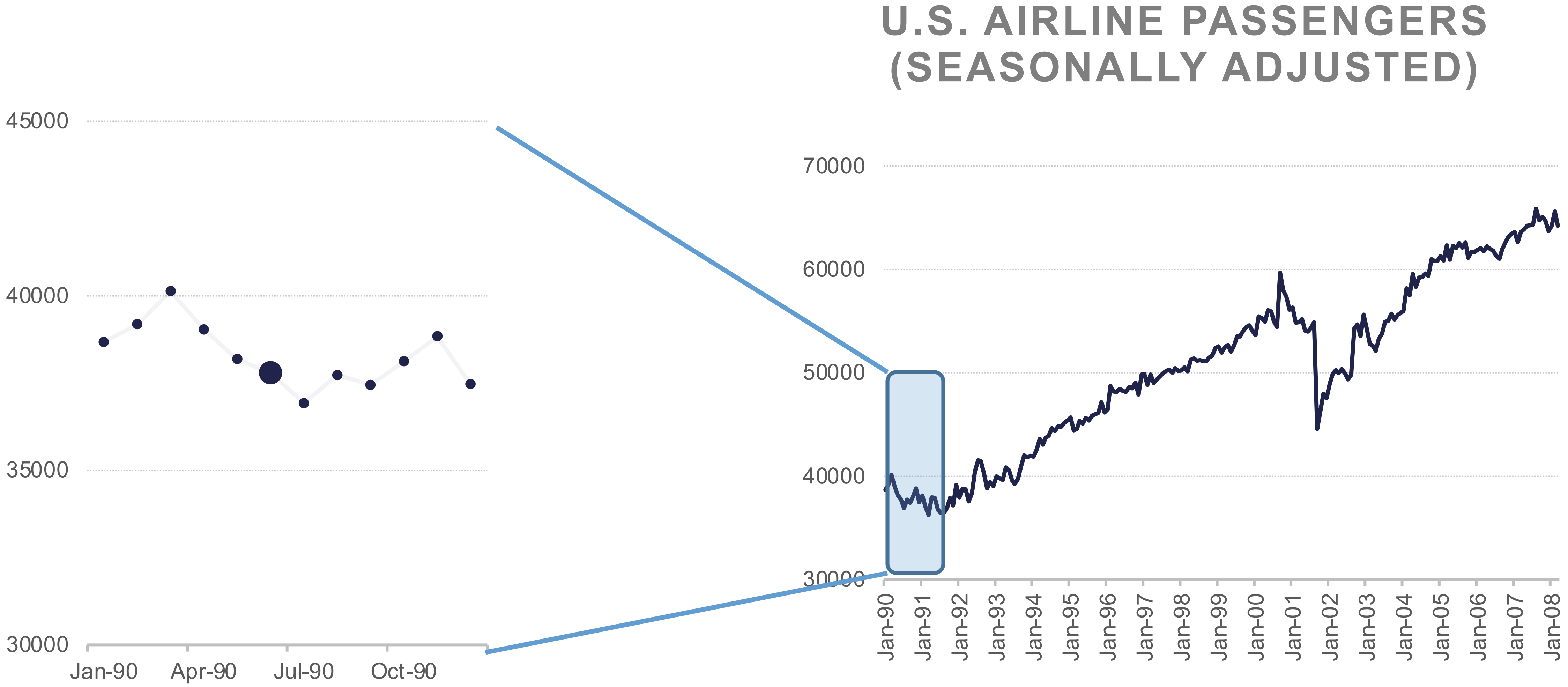
LOESS

- Locally estimated scatterplot smoothing (LOESS) is a popular smoothing technique.
- Same technique used in STL decomposition in time series

LOESS


U.S. AIRLINE PASSENGERS (SEASONALLY ADJUSTED)
45000
40000
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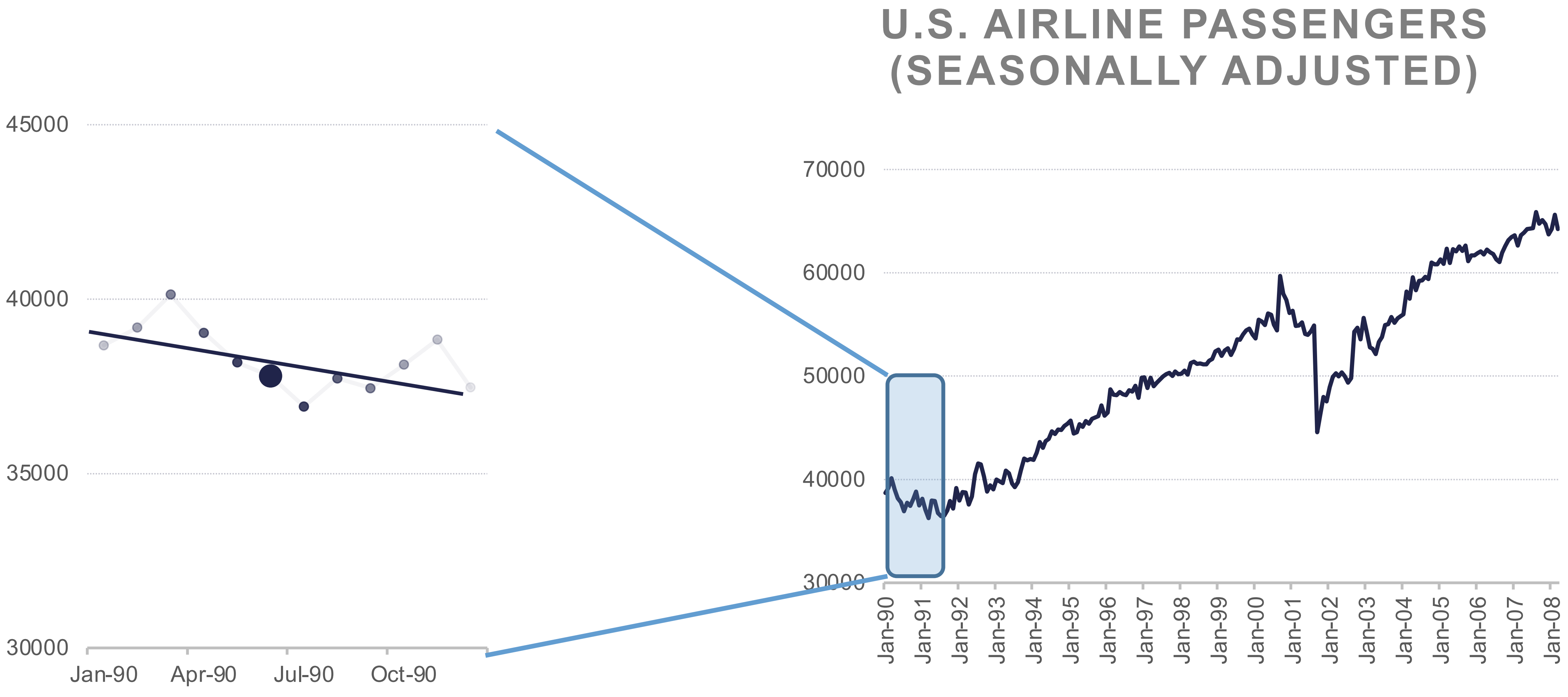
LOESS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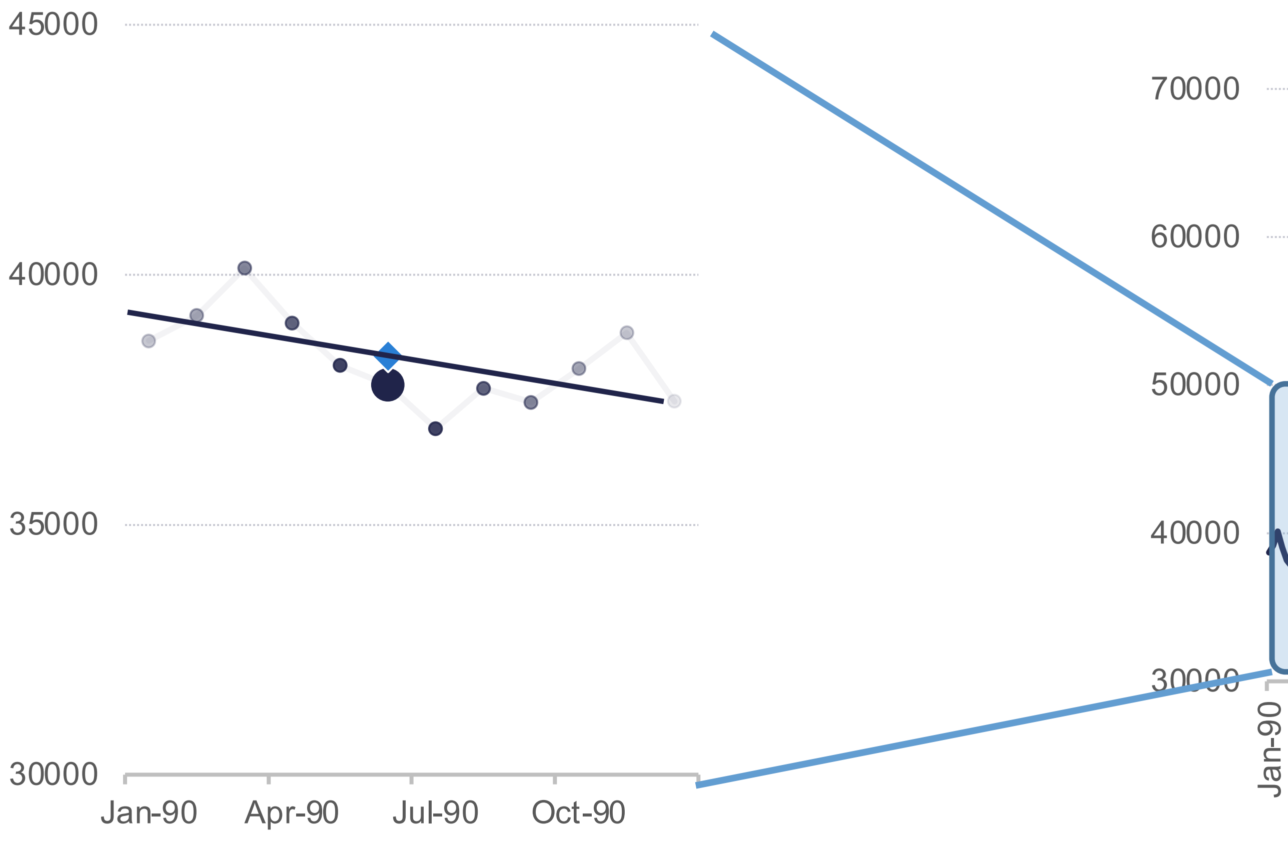
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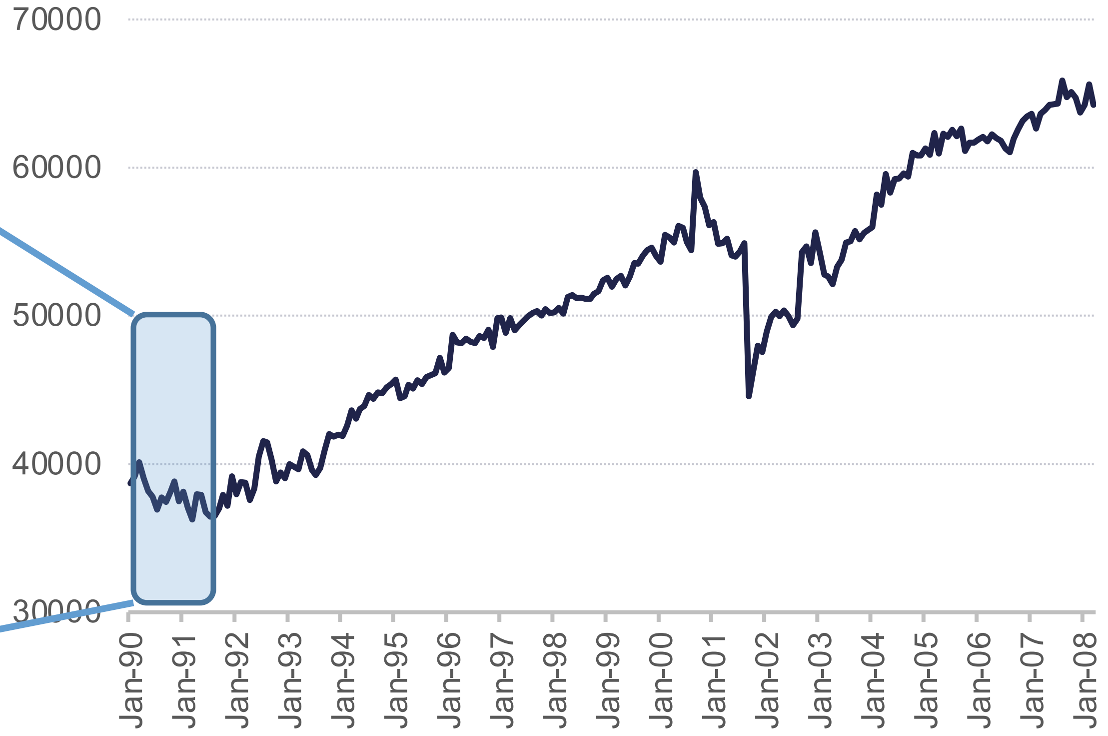
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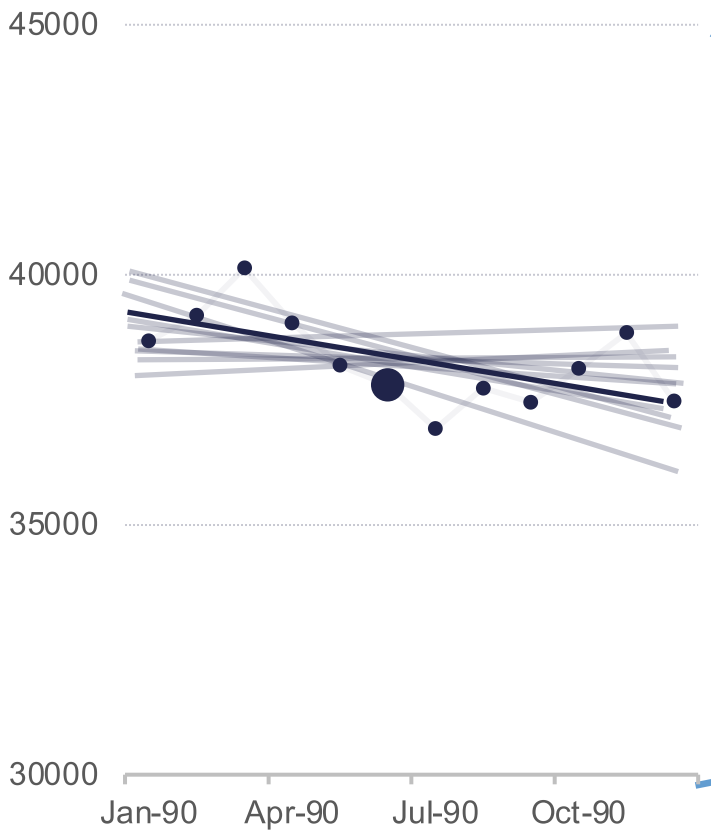
LOESS



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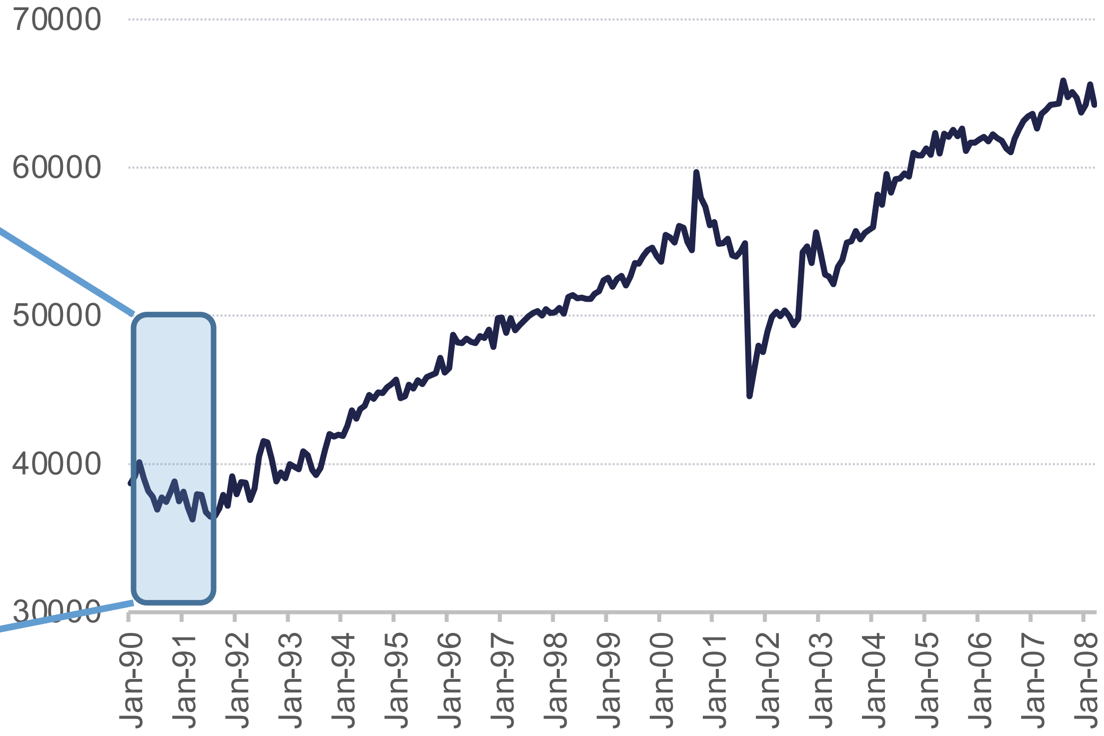

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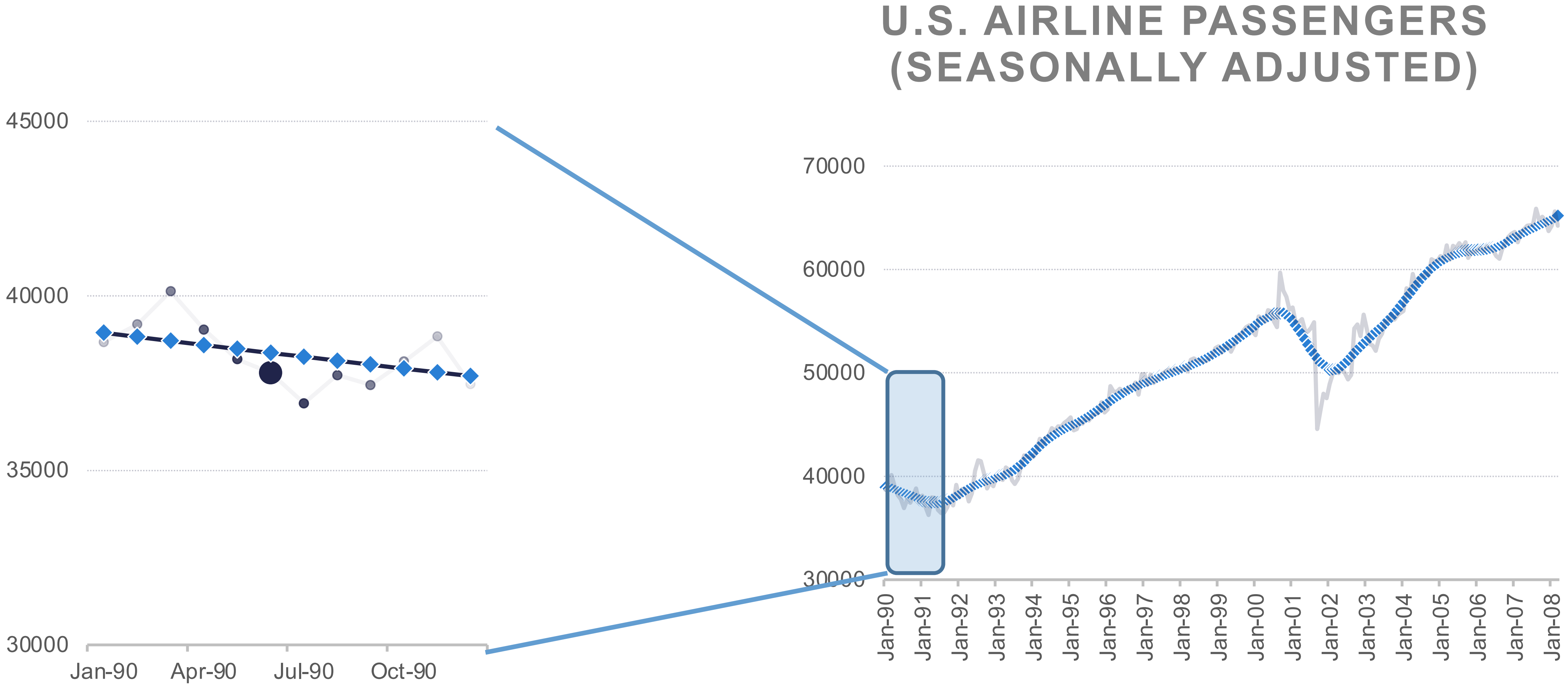
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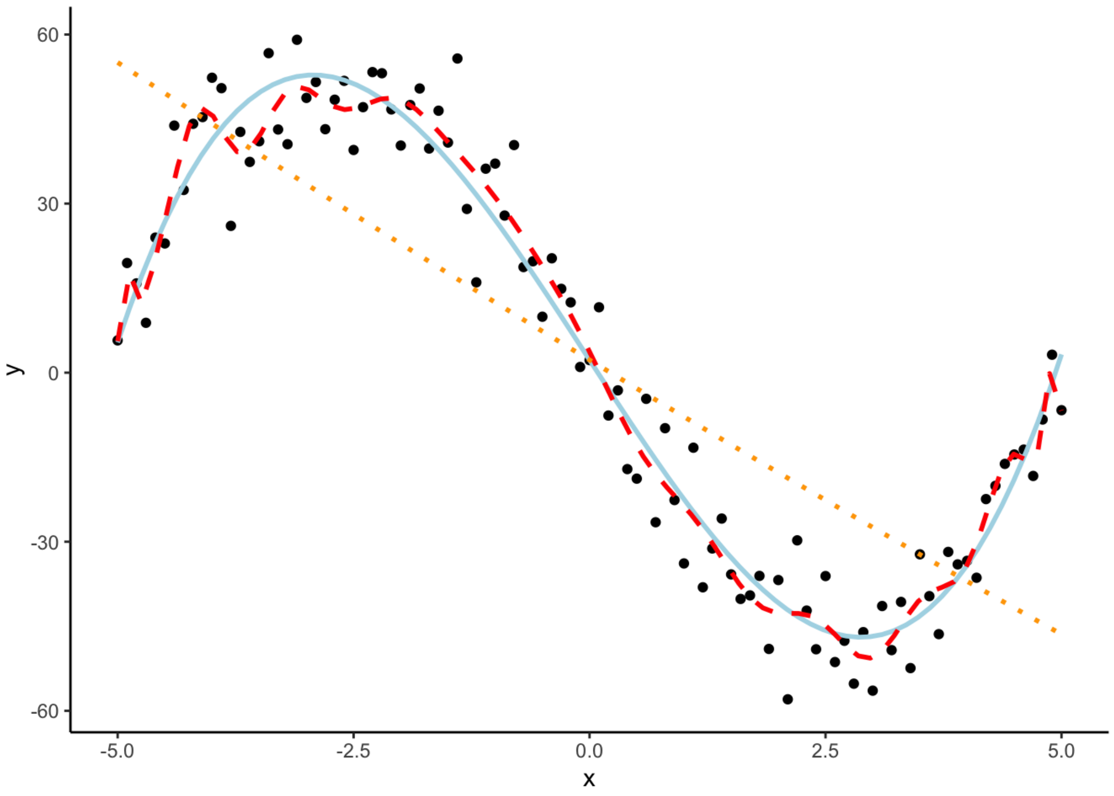
Smoothing

- GAMs can be made up of any non-parametric function of the predictor variables.
- Another popular technique is to use **smoothing functions** so the piecewise linear regressions are not so jagged.
- Many different types of smoothing functions:
  - LOESS (localized regression)
  - Smoothing splines
  - Regression splines

Smoothing Splines

- Smoothing splines take a different approach as compared to LOESS.
- Smoothing splines have a knot **at every single observation** for piecewise regression – OVERFITTING!
- Use penalty parameter to counterbalance the “wiggle” of the spline.



Smoothing Splines

- Smoothing splines try to find the function $s(x_i)$ that optimally fits *x* to the target variable *y* through this equation:

$$\min \sum_{i=1}^{n} \left(y_i - s(x_i)\right)^2 + \lambda \int s''(t_i)^2 \, dt$$

Smoothing Splines

- Smoothing splines try to find the function $s(x_i)$ that optimally fits *x* to the target variable *y* through this equation:

$$\min \boxed{\sum_{i=1}^{n} \left(y_i - s(x_i)\right)^2} + \lambda \int s''(t_i)^2 \, dt$$

Sum of squared error!

Smoothing Splines

- Smoothing splines try to find the function $s(x_i)$ that optimally fits *x* to the target variable *y* through this equation:

$$\min \sum_{i=1}^{n} \left(y_i - s(x_i)\right)^2 + \boxed{\lambda \int s''(t_i)^2 \, dt}$$

Penalty (λ) applied to integral of second derivative of smoothing function

Smoothing Splines

- Smoothing splines try to find the function $s(x_i)$ that optimally fits *x* to the target variable *y* through this equation:

$$\min \sum_{i=1}^{n} \left(y_i - s(x_i)\right)^2 + \boxed{\lambda \int s''(t_i)^2 \, dt}$$

Penalty (λ) applied to integral of "slope of slopes" which is large when lots of "wiggle"

Smoothing Splines

- Smoothing splines try to find the function $s(x_i)$ that optimally fits *x* to the target variable *y* through this equation:

$$\min \sum_{i=1}^{n} \left(y_i - s(x_i)\right)^2 + \boxed{\lambda} \int s''(t_i)^2 \, dt$$

Penalty (λ) estimated with another approximation of leave one out cross validation

Smoothing

- GAMs can be made up of any non-parametric function of the predictor variables.
- Another popular technique is to use **smoothing functions** so the piecewise linear regressions are not so jagged.
- Many different types of smoothing functions:
  - LOESS (localized regression)
  - Smoothing splines
  - Regression splines – computationally nicer version of smoothing splines

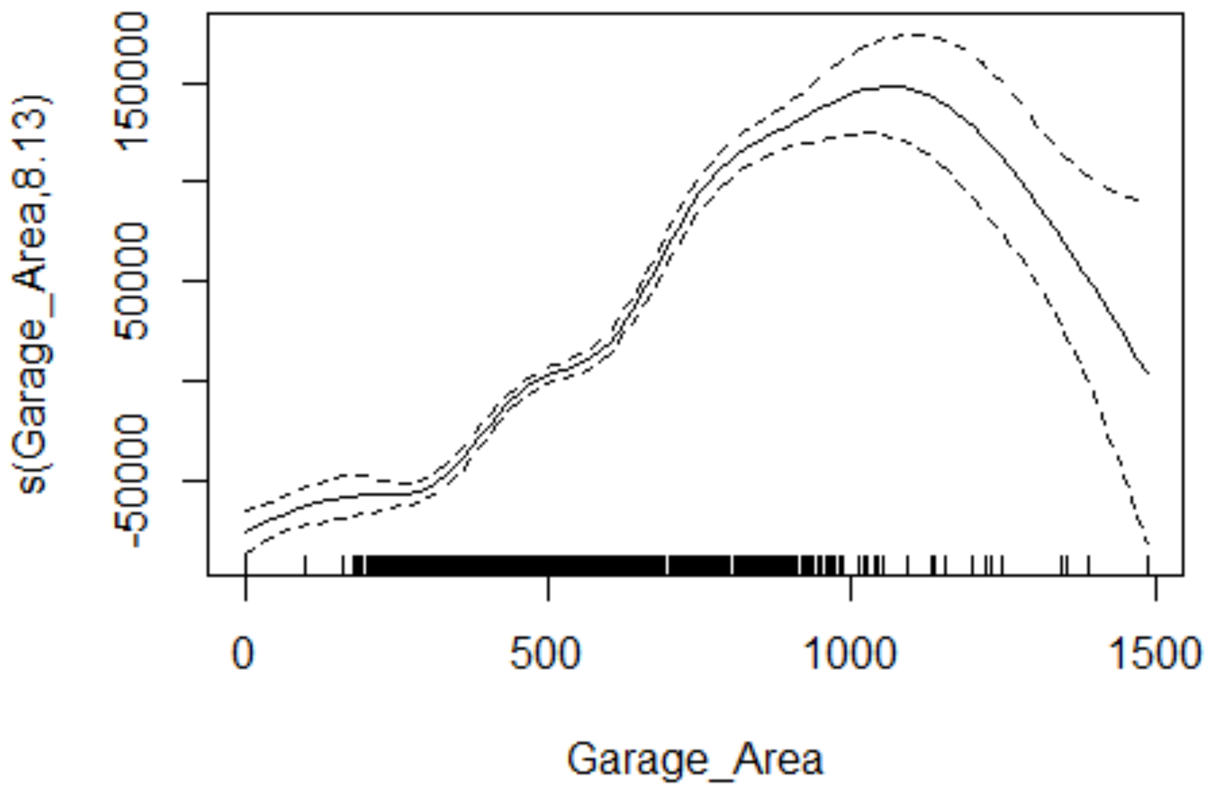
GAM's with Splines

```
gam1 <- mgcv::gam(Sale_Price ~ s(Garage_Area), data = training)
summary(gam1)
```

```
## Family: gaussian
## Link function: identity
##
## Formula:
## Sale_Price ~ s(Garage_Area)
##
## Parametric coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   180897       1290   140.2   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Approximate significance of smooth terms:
##                  edf Ref.df     F p-value
## s(Garage_Area) 8.134  8.769 192.5  <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) =  0.451   Deviance explained = 45.3%
## GCV = 3.4301e+09  Scale est. = 3.4148e+09  n = 2051
```

GAM's with Splines

```
plot(gam1)
```



GAM's with Splines

```
gam2 <- mgcv::gam(Sale_Price ~ s(Bedroom_AbvGr, k = 5) +
                               s(Year_Built) +
                               s(Mo_Sold) +
                               s(Lot_Area) +
                               s(First_Flr_SF) +
                               s(Second_Flr_SF) +
                               s(Garage_Area) +
                               s(Gr_Liv_Area) +
                               s(TotRms_AbvGrd) +
                               Street +
                               Central_Air +
                               factor(Fireplaces) +
                               factor(Full_Bath) +
                               factor(Half_Bath)
                  , method = 'REML', data = training)
summary(gam2)
```

GAM's with Splines

```
## Parametric coefficients:
##                      Estimate Std. Error t value Pr(>|t|)    
## (Intercept)            136139      19681   6.917 6.19e-12 ***
## StreetPave              27689      12710   2.178   0.0295 *  
## Central_AirY            18012       3168   5.685 1.50e-08 ***
## factor(Fireplaces)1     14070       1666   8.443  < 2e-16 ***
## factor(Fireplaces)2     27137       3146   8.626  < 2e-16 ***
## factor(Fireplaces)3     15704      10552   1.488   0.1368    
## factor(Fireplaces)4    -79595      31469  -2.529   0.0115 *  
## factor(Full_Bath)1      -5341      14528  -0.368   0.7132    
## factor(Full_Bath)2     -11074      14827  -0.747   0.4552    
## factor(Full_Bath)3       1226      15787   0.078   0.9381    
## factor(Full_Bath)4     -16271      24326  -0.669   0.5037    
## factor(Half_Bath)1       2102       2206   0.953   0.3408    
## factor(Half_Bath)2     -38507       9111  -4.226 2.48e-05 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
...
```

GAM’s with Splines

```
...
## Approximate significance of smooth terms:
##                     edf Ref.df       F p-value    
## s(Bedroom_AbvGr) 2.653  3.165  18.789  <2e-16 ***
## s(Year_Built)    6.445  7.543 101.758  <2e-16 ***
## s(Mo_Sold)       1.516  1.868   0.993  0.4507    
## s(Lot_Area)      7.186  8.193  11.726  <2e-16 ***
## s(First_Flr_SF)  8.063  8.765  15.548  <2e-16 ***
## s(Second_Flr_SF) 8.212  8.818   7.806  <2e-16 ***
## s(Garage_Area)   7.426  8.328  21.654  <2e-16 ***
## s(Gr_Liv_Area)   8.545  8.882  14.834  <2e-16 ***
## s(TotRms_AbvGrd) 3.805  4.738   1.921  0.0783 .  
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) =  0.851   Deviance explained = 85.6%
## -REML =  23957  Scale est. = 9.2392e+08  n = 2051
```

GAM's with Selected Splines

```
sel.gam2 <- mgcv::gam(Sale_Price ~ s(Bedroom_AbvGr, k = 5) +
                                   s(Year_Built) +
                                   s(Mo_Sold) +
                                   s(Lot_Area) +
                                   s(First_Flr_SF) +
                                   s(Second_Flr_SF) +
                                   s(Garage_Area) +
                                   s(Gr_Liv_Area) +
                                   s(TotRms_AbvGrd) +
                                   Street +
                                   Central_Air +
                                   factor(Fireplaces) +
                                   factor(Full_Bath) +
                                   factor(Half_Bath)
                        , method = 'REML',
                          select = TRUE, data = training)
summary(sel.gam2)
```

```
## Approximate significance of smooth terms:
##                       edf Ref.df      F  p-value
## s(Bedroom_AbvGr) 2.333381      4 14.833  < 2e-16 ***
## s(Year_Built)    6.945994      9 83.962  < 2e-16 ***
## s(Mo_Sold)       0.007522      9  0.001  0.33142
## s(Lot_Area)      7.561273      9 11.790  < 2e-16 ***
## s(First_Flr_SF)  8.602695      9 32.390  < 2e-16 ***
## s(Second_Flr_SF) 0.940878      9  1.716 3.89e-06 ***
## s(Garage_Area)   6.688676      9 19.626  < 2e-16 ***
## s(Gr_Liv_Area)   4.839941      9  7.634  < 2e-16 ***
## s(TotRms_AbvGrd) 3.740058      9  1.280  0.00845 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## R-sq.(adj) =  0.845   Deviance explained = 84.9%
## -REML =  24081  Scale est. = 9.6657e+08  n = 2051
```

SUMMARY

Generalized Additive Models (GAMs)

- Provides **general** framework for **adding** of non-linear functions together instead of the typical linear structure.

$$y = \beta_0 + f_1(x_1) + f_2(x_2) + \cdots + f_p(x_p) + \varepsilon$$

- Can be used for regression or classification problems.

Generalized Additive Models (GAMs)

Advantages

- Allows a nonlinear relationship without trying out many transformations manually
- Improved predictions
- Still has some “interpretation”
- Computationally fast

Disadvantages

- Can incorporate interactions but can take time
- Not good for large numbers of variables – **prescreening needed!**
- Multicollinearity still a problem

?