Answers in Multivariate Adaptive Regression Splines (MARS)

BC2407 ANALYTICS II SEMINAR 6

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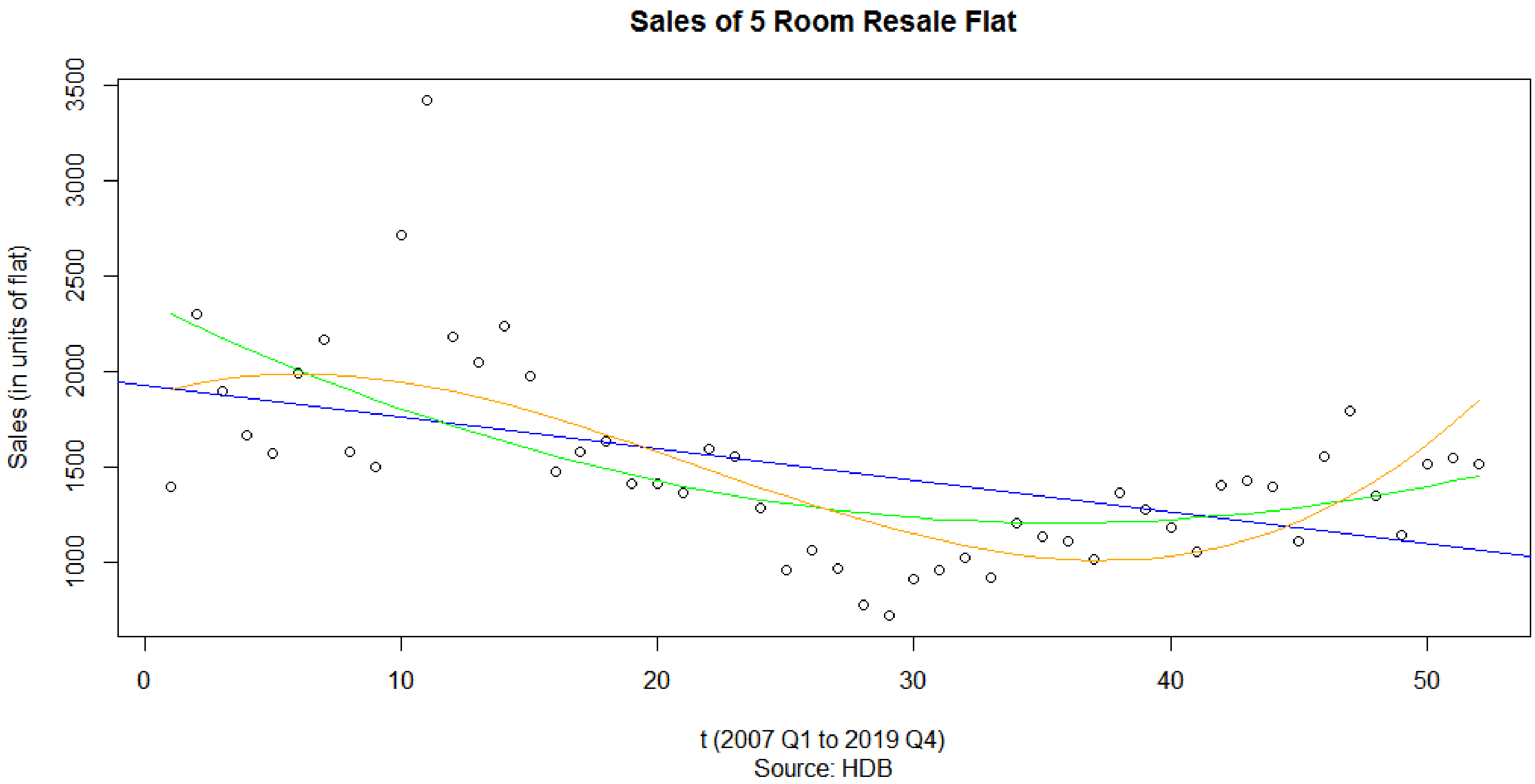
Fitted Linear, Quadratic and Cubic Trends



- What is the problem with using Linear/Quadratic/Cubic reg?
- Ans: The trend applies globally throughout the data.

```
> m.mars1$coefficients
              Sales.5rm
(Intercept) 3994.20425
h(t-32)       96.05913
h(32-t)      -77.57353
h(t-11)     -172.75760
h(t-26)      105.03626
```

Hinge functions in MARS

- The Mars model is a weighted combination of hinge functions:
- $\hat{y} = 3994.2 - 172.8\mathrm{h}(\mathrm{t} - 11) + 105\mathrm{h}(\mathrm{t} - 26) + 96.1\mathrm{h}(\mathrm{t} - 32) - 77.6\mathrm{h}(32 - \mathrm{t})$
- Hinge function: h(s) ≡ max(s, 0).
- Q: What is the MARS model predicted value of y if
  - t = 10
  - t = 20
  - t = 40

Answers

- At t = 10: $\hat{y} = 3994.2 - 172.8(0) + 105(0) + 96.1(0) - 77.6(22) = 2287$

- At t = 20: $\hat{y} = 3994.2 - 172.8(9) + 105(0) + 96.1(0) - 77.6(12) = 1507.8$

- At t = 40: $\hat{y} = 3994.2 - 172.8(29) + 105(14) + 96.1(8) - 77.6(0) = 1221.8$

FAQ: Why trace reveal only one pair added in forward pass?

```
         GRSq    RSq     DeltaRSq Pred      PredName        Cut  Terms    Par Deg
1      0.0000 0.0000                      (Intercept)
2      0.3979 0.4886       0.4886    1              t        32  2   3          1
4      0.5455 0.6461       0.1575    1              t        11  4              1
6      0.5731 0.6965      0.05038    1              t        26  5              1
8      0.5340 0.6988     0.002353    1              t        38  6              1
10     0.4857 0.6992    0.0003907    1              t        41  7              1 reject (small DeltaRSq)
```

Ans: This is another different implementation compared to theory. In R earth-notes documentation p.6:

" the forward pass discards one side of a term pair if it adds nothing to the model — but the forward pass counts terms as if they were actually created in pairs,"

i.e. after the first pair is added (checking that each term in the pair contributes significantly to reducing RSS), the future pairs are actually added solo as the other side was checked and found to contribute "nothing" to reducing RSS. For software, we need to set a threshold to define "nothing" e.g. less than 0.0000001 for RSS or < 0.001 for Rsq

Overview of MARS Model Development

Initialize MARS → Grow MARS → Prune MARS

- Similar strategy to CART.
- Grow to add the “best” hinge (in reflected pairs) at each step.
- Prune to remove weakest hinge terms when complexity penalty is included to reduce risk of overfitting; Remove one term per step.
- Note: Implementation differences with different software.

MARS Implementation in R earth() vs Python py-earth

Initialize MARS

- Choose degree. Default = 1.
- Choose pruning method (GRsq , GCV or k-fold CV).
- R Default : GRsq.
- Python Default: GCV.

Grow MARS

- Add the "best" hinge functions in reflected pairs, one pair per step.
- Best determined by largest increase in Rsq (R) or largest decrease in RSS (Python) to current model.
- Update current model coefs by lm fit, after each addition.
- Stop when Rsq increase < 0.001 or no new term increases Rsq.

Prune MARS

- Remove weakest term, one at each step.
- The weakest term defined as the term whose removal result in smallest increase in RSS.
- Compute complexity adjusted model error GRsq, GCV or mean OOF CV error.
- Use GRSq, GCV, or k-fold CV to estimate optimal number of terms in final model.

"The GRSq normalizes the GCV in the same way that the Rsq normalizes the RSS".
– R earth notes documentation p.29

GCV and GRsq
Source: earth notes documentation p.57.

$$\text{GCV = RSS / (n * (1 - nparams / n)^2))}$$

Effective Number of Parameters in MARS

$$\text{GRSq = 1 - GCV / GCV.null,}$$

where GCV.null is the GCV of an intercept-only model.

- GCV actually adjust the RSS to account for model complexity i.e. complexity adjusted RSS. No Cross Validation is used.
- Both GCV and GRsq are opinionated estimation of model predictive performance on future unseen data, by adding a penalty for model complexity (number of hinges in MARS).
- GRSq is the normalized version of GCV, scaled to between 0 to 1 under normal conditions.
- A means for more direct-than-k-fold CV estimation of testset error.

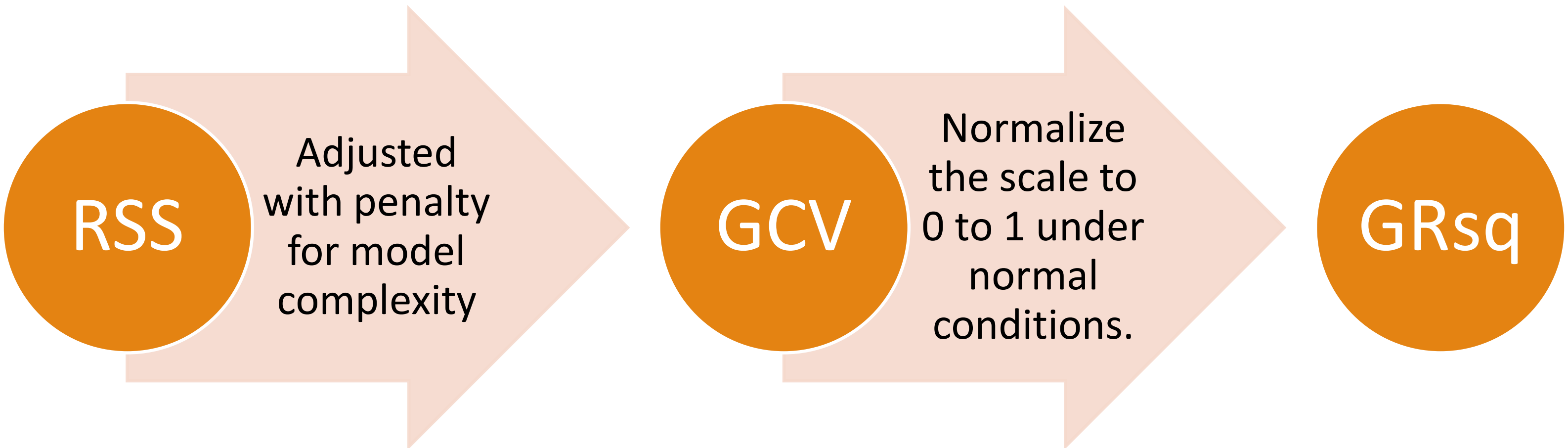
FAQ: How to compute nparams?

Effective number of parameters =

(num of terms) + (penalty) * ½ (num of terms − 1)

- num of terms – 1 is the number of hinge terms
- Take ½ to compensate for double counting of terms added in pairs during forward pass.

FAQ: What's the relationship between RSS, GCV, GRsq?



- RSS has no penalty for model complexity and thus will select the most complex model as RSS will be lowest.
- GCV and GRsq are ways to incorporate penalty for model complexity into RSS. Using either will select a model neither too big nor too small, and thus avoid overfitting. Substitute for 10-fold CV.

Pruning alternative using 10-fold CV

- Default in earth():
  - nfold = 0
  - ncross = 1
- 10-fold CV: set nfold = 10
- Since CV is sensitive to data partition, try ncross > 3, to repeat 10-fold CV multiple times with another random partition of data.
- CVRsq is the mean Rsq from out-of-fold (OOF) data.
  - Note: CVRsq still use terms selected by GCV – earth notes p.38
- Use pmethod = "cv" to select the select optimal model using cross-validation.
  - Based on max mean OOF Rsq, not 1SE rule.

Class Activity 1

Single Variate MARS

Est. Duration: 30 mins

1. Run flatsales-mars.R
2. What is the MARS model coefficients and RMSE if 10-fold CV is used to prune instead of GRsq? Which ncross level is more stable?
   - Seed = 2 vs 2020
   - pmethod="cv“
   - nfold = 10
   - ncross = 1 vs 5

Instructor answers in flatsales-mars2.R will be posted by end of week.

Class Activity 1

Single Variate MARS

Est. Duration: 30 mins

3. Create a copy of the sales dataset as an Excel workbook. Using Excel, show that the linear regression model with the selected 4 hinge functions has the same model coefficients as R output.

4. Advanced option: Compute GCV, GCV.null and GRsq in excel.

Instructor answers in 5 room flat resale applications solution.xlsx will be posted by end of week.

```
> summary(m.mars1)
Call: earth(formula=Sales.5rm~t, data=data.sales, degree=1)

              coefficients
(Intercept)      3994.2043
h(t-11)          -172.7576
h(t-26)           105.0363
h(32-t)           -77.5735
h(t-32)            96.0591

Selected 5 of 6 terms, and 1 of 1 predictors
Termination condition: RSq changed by less than 0.001 at 6 terms
Importance: t
Number of terms at each degree of interaction: 1 4 (additive model)
GCV 109300    RSS 3886456    GRSq 0.5730591    RSq 0.696496
```

Answers to Class Activity 1

- Q2: ncross = 5 is more stable than ncross = 1 as MARS Model and RMSE remains the same despite change in seed. [See RScript solution.] This shows CV is sensitive to data partition.
- Q3: See workings and solution in excel file solution.

	A	B	C	D	E
1	SUMMARY OUTPUT				
2					
3	*Regression Statistics*			MARS	
4	Multiple R	0.834563		Eff nparams	9
5	R Square	0.696496		GCV	109300.01
6	Adjusted R Square	0.670666		GCV.null	256007.34
7	Standard Error	287.5597		GRsq	0.5730591
8	Observations	52			
9					
10	ANOVA				
11		*df*	*SS*	*MS*	*F*
12	Regression	4	8918834	2229708.51	26.964488
13	Residual	47	3886456.2	82690.5572	
14	Total	51	12805290		
15					
16		*Coefficients*	*Standard Error*	*t Stat*	*P-value*
17	Intercept	3994.204	538.99859	7.41041691	1.956E-09
18	h(t-11)	-172.758	30.585599	-5.6483314	9.131E-07
19	h(t-26)	105.0363	37.603984	2.7932216	0.0075262
20	h(32-t)	-77.5735	21.552891	-3.59921689	0.0007656
21	h(t-32)	96.05913	38.009446	2.52724351	0.0149191

Class Activity 2

Multi-Variate MARS

Est. Duration: 30 mins

1. Create a new continuous X variable remaining lease in years.
2. Change the Baseline Reference level for Town to Yishun instead of default.
3. Use only the 4 main Xs stated previously.
4. Develop 2 MARS models and compare their RMSE and model coefficients.
   - degree = 1
   - degree = 2
5. Using the 2 MARS models, predict the resale price of a flat in Clementi, 100 square metres, 19-21 storey & 80 yrs lease remaining. Verify your calculations using hinge functions in Excel.
6. Which X variables are relatively more impt in MARS degree 2 model?

Instructor answers in flatprice-mars solution.R & flatprice-mars predictions.xlsx will be posted by end of week.

Python Implementation of MARS

- py-earth
  - https://github.com/scikit-learn-contrib/py-earth
  - Learnt from R earth package.
  - Incl. missing data support (R earth has no support for NAs).
  - Some Differences in py-earth compared to R earth:
    - Penalty = 3 (In R earth, penalty = 2 for additive model, 3 otherwise.)
    - Use MSE (i.e. same as using RSS) in forward pass (R earth use Rsq)
    - Use GCV in pruning pass (R earth use GRsq)
    - Did not discard any term during forward pass (R earth may discard terms)
    - Others…

Python code for HDB 5-rm Sales data

```
from pyearth import Earth
import pandas as pd

df = pd.read_csv (r'D:/Dropbox/Datasets/HDB Resale Prices/subset2017-19/5 room flat resale applications.csv')
df['t'] = pd.Series(range(1,53))
```

```
mars = Earth(penalty=2)
mars.fit(X=df['t'], y=df['Sales 5rm'])
print(mars.summary())
## Result is not the same as R. Different implementation?
## Increase max_terms does not craete more terms as threshold reached.
```

```
Earth Model
-------------------------------------
Basis Function  Pruned  Coefficient
-------------------------------------
(Intercept)     No      392.019
h(x0-29)        Yes     None
h(29-x0)        No      113.126
h(x0-12)        Yes     None
h(12-x0)        No      -173.099
h(x0-16)        No      33.9763
h(16-x0)        Yes     None
x0              Yes     None
-------------------------------------
MSE: 75943.3561, GCV: 101407.8197, RSQ: 0.6916, GRSQ: 0.6039
```

Recall from BC2406:
There is often more than one correct model.
It's fine to use this MARS but be aware of the differences between Python vs R implementations.

Trace py-earth MARS reveals different criteria compared to R earth

```
print(mars.trace())
```

```
Forward Pass
--------------------------------------------------------------------------
iter  parent  var  knot  mse            terms  gcv          rsq    grsq
--------------------------------------------------------------------------
0     -       -    -     246255.581361  1      256007.340   0.000  0.000
1     0       0    28    126746.046454  3      155147.718   0.485  0.394
2     0       0    11    79422.110668   5      116147.857   0.677  0.546
3     0       0    15    71450.868851   7      127023.767   0.710  0.504
4     0       0    -1    71450.868851   8      141127.209   0.710  0.449
--------------------------------------------------------------------------
Stopping Condition 2: Improvement below threshold

Pruning Pass
------------------------------------------------------
iter  bf  terms  mse        gcv         rsq    grsq
------------------------------------------------------
0     -   8      71450.87   141127.209  0.710  0.449
1     7   7      71450.87   127023.767  0.710  0.504
2     6   6      71450.87   114933.462  0.710  0.551
3     1   5      71450.87   104490.616  0.710  0.592
4     3   4      75943.36   101407.820  0.692  0.604
5     5   3      115080.20  140867.751  0.533  0.450
6     4   2      141750.54  159639.094  0.424  0.376
7     2   1      246255.58  256007.340  0.000  0.000
------------------------------------------------------
Selected iteration: 4
```

Note the inconsistency in term names and knots between the summary() results and trace().