

Model Selection

Institute for Advanced Analytics MSA Class of 2025

Review of Modeling Up Until Now...

- Simple Linear Regression one predictor variable for continuous target.
- Multiple Linear Regression many predictor variables (continuous or categorical) for continuous target.
- With many explanatory variables, how do we know which ones are most informative?

Ames Housing Data

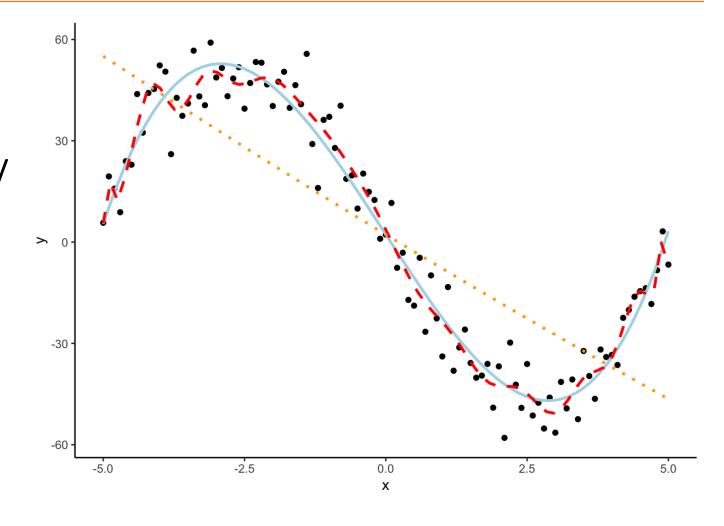
- Sale Price predicted with...
 - Greater Living Area
 - Lot Size
 - Central Air
 - Heating Quality
 - Number of Rooms
 - Number of Bathrooms
 - And many, many, more...

Model Building Concepts

- Information Criteria commonly used to "select" variables for the model.
- Selection Algorithm automated technique to quickly evaluate variables based on some selection criteria.
 - Stepwise Selection (forward, backward, stepwise)
 - All-regression Selection (R^2 , R_a^2 , Mallow's C_p)

Fear of Overfitting

- Model selection should always be done with training data.
- Will hold out validation / testing data to help evaluate (honest assessment) if we have overfit our data.
- In machine learning, we will use cross-validation.





Information Criteria

AIC and BIC

- AIC and BIC approximate out-of-sample prediction error by applying a penalty for model complexity:
 - AIC (Akaike Information Criterion) crude, large-sample approximation of leave-one-out cross-validation.
 - BIC (Bayesian Information Criterion) favors smaller models/penalizes model complexity more.
- Lower values "better" than higher.
- No amount of lower is "better" enough.
- May not always agree, but neither is necessarily better.

AIC and BIC

AIC (Akaike Information Criterion)

$$AIC = -2\log(L) + 2k$$

$$AIC = n\log\left(\frac{SSE}{n}\right) + 2k$$

• BIC (Bayesian Information Criterion)

BIC =
$$-2 \log(L) + k \log(n)$$

BIC = $n \log\left(\frac{SSE}{n}\right) + k \log(n)$

AIC and BIC

AIC (Akaike Information Criterion)

$$AIC = -2\log(L) + 2k$$

$$AIC = n\log\left(\frac{SSE}{n}\right) + 2k$$

• BIC (Bayesian Information Criterion)

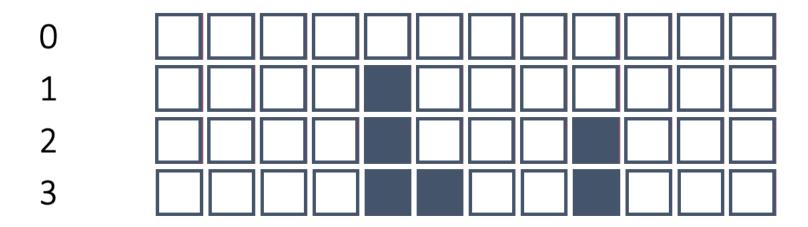
BIC =
$$-2 \log(L) + k \log(n)$$

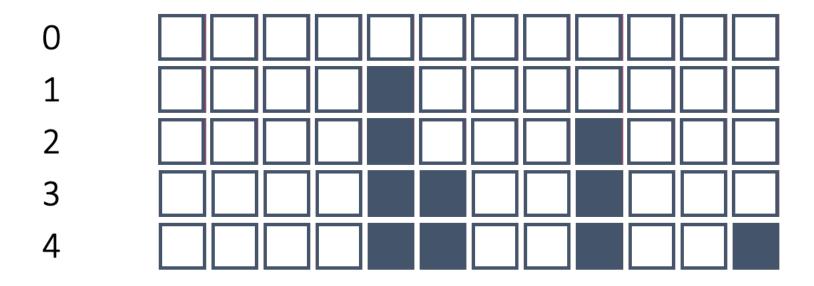
BIC = $n \log\left(\frac{SSE}{n}\right) + k \log(n)$

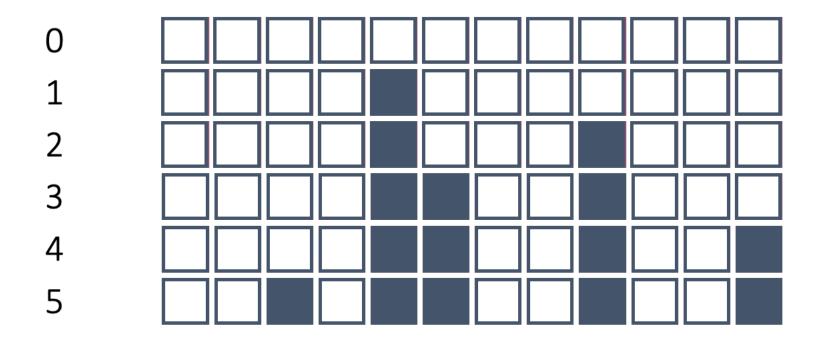
- Start with a "null" model (just the intercept) and systematically build the model (one variable at a time).
- 1. Start with intercept only model (this is the base model)
- 2. For each variable not in model, create a linear regression model with the base model plus this variable
- 3. See which linear regression is best (based on criterion)
- 4. If better than base model, continue to next step... otherwise STOP (this is your model)
- 5. Update base model to this new model, repeat whole process...

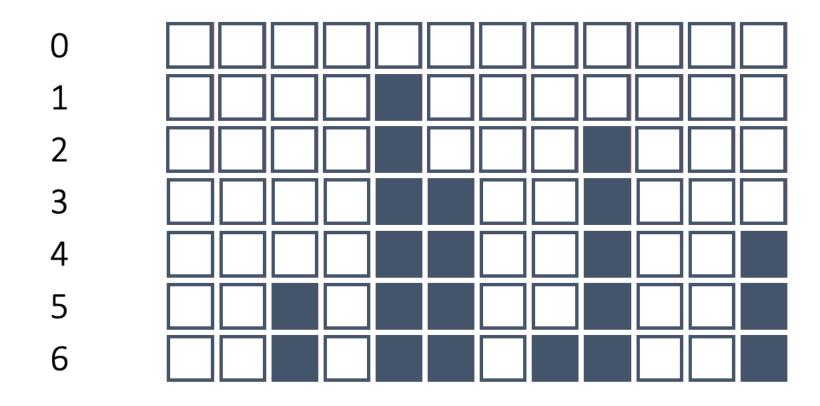


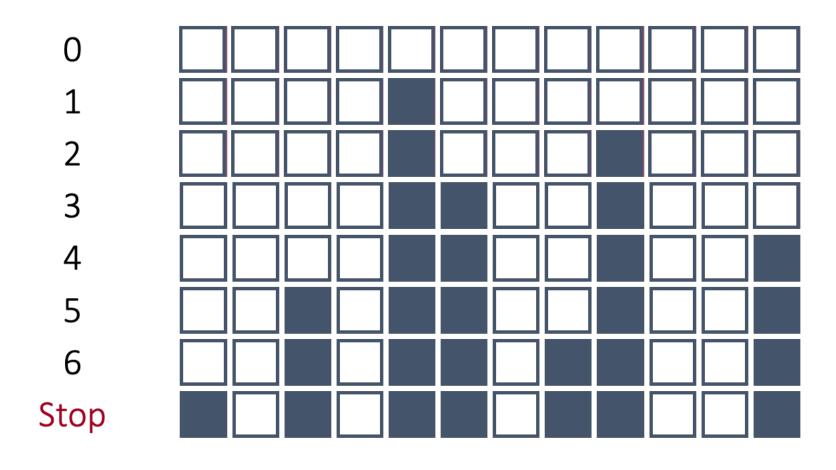












Selecting Some Variables

Selecting Some Variables

Replacing all missing with mean of the column for now. Will discuss different imputations at later date!

Start: AIC=46323.64 Sale Price ~ 1

- Step 1
- AIC from base model at top of output.
- Shows the addition ("+")
 of each variable and the
 "new" AIC from that
 model.
- Best variable at top.

```
Sum of Sq
                                    RSS
                                           AIC
                 9 9.3437e+12 3.8531e+12 43817
+ Overall Qual
+ Gr Liv Area
                 1 6.4389e+12 6.7578e+12 44953
                 1 5.3561e+12 7.8407e+12 45258
+ Garage Area
+ First Flr SF
                 1 4.8867e+12 8.3100e+12 45377
+ Full Bath
                 1 3.7827e+12 9.4141e+12 45633
+ TotRms AbvGrd
                 1 3.2304e+12 9.9663e+12 45750
+ Fireplaces
                 1 2.9715e+12 1.0225e+13 45802
+ Half Bath
                 1 1.1209e+12 1.2076e+13 46144
+ Roof Style
                 5 1.0724e+12 1.2124e+13 46160
+ Central Air
                 1 9.6147e+11 1.2235e+13 46170
+ House Style
                 7 1.0245e+12 1.2172e+13 46172
+ Second Flr SF
                 1 9.4611e+11 1.2251e+13 46173
+ Lot Area
                 1 9.0332e+11 1.2293e+13 46180
                 4 4.6434e+11 1.2732e+13 46258
+ Bldg Type
+ Street
                 1 3.1752e+10 1.3165e+13 46321
                              1.3197e+13 46324
<none>
```

Step: AIC=43816.66
Sale Price ~ Overall Qual

- Step 2
- AIC from new base model at top of output.
- Shows the addition ("+")
 of each variable and the
 "new" AIC from that
 model.
- Best variable at top.
- Notice the <none>...

```
Sum of Sq
                                    RSS
                                          AIC
                1 9.8905e+11 2.8640e+12 43210
+ Gr Liv Area
+ First Flr SF
                1 5.2665e+11 3.3264e+12 43517
                1 4.6644e+11 3.3866e+12 43554
+ Garage Area
+ TotRms AbvGrd
                1 4.6123e+11 3.3918e+12 43557
+ Full Bath
                1 4.1206e+11 3.4410e+12 43587
                1 4.0551e+11 3.4476e+12 43591
+ Fireplaces
                1 3.8148e+11 3.4716e+12 43605
+ Lot Area
+ Bldg Type
                 4 2.3715e+11 3.6159e+12 43694
+ Second Flr SF
                1 1.7555e+11 3.6775e+12 43723
+ Half Bath
                1 1.3948e+11 3.7136e+12 43743
+ Central Air
                1 9.1322e+10 3.7617e+12 43769
+ House Style
                7 6.1815e+10 3.7912e+12 43797
+ Roof Style
                5 5.1448e+10 3.8016e+12 43799
                             3.8531e+12 43817
<none>
                1 1.9573e+06 3.8531e+12 43819
+ Street
```

Step: AIC=43210.24
Sale_Price ~ Overall_Qual + Gr_Liv_Area

- Step 3
- AIC from new base model at top of output.
- Shows the addition ("+")
 of each variable and the
 "new" AIC from that
 model.
- Best variable at top.
- Watch the <none>...

```
Sum of Sq
                                    RSS
                                          AIC
                7 2.5351e+11 2.6105e+12 43034
+ House Style
                1 2.1638e+11 2.6476e+12 43051
+ Garage Area
                1 1.3097e+11 2.7330e+12 43116
+ Lot Area
+ First Flr SF
                1 1.2210e+11 2.7419e+12 43123
+ Fireplaces
                1 1.1069e+11 2.7533e+12 43131
+ Central Air
                1 1.1050e+11 2.7535e+12 43132
+ Second Flr SF
                1 1.0207e+11 2.7619e+12 43138
+ Bldg Type
                4 1.0299e+11 2.7610e+12 43143
+ Roof Style
                5 6.0726e+10 2.8033e+12 43176
+ Full Bath
                1 3.2970e+10 2.8310e+12 43188
                1 2.4688e+10 2.8393e+12 43194
+ TotRms AbvGrd
<none>
                             2.8640e+12 43210
+ Half Bath
                1 4.0261e+07 2.8640e+12 43212
                1 2.2632e+07 2.8640e+12 43212
+ Street
```

- Step 15
- Exit the algorithm since <none> is the highest step.
- Poor Street variable...

```
Step: AIC=42676.1
Sale_Price ~ Overall_Qual + Gr_Liv_Area +
House_Style + Garage_Area + Bldg_Type +
Fireplaces + Full_Bath + Half_Bath + Lot_Area +
Roof_Style + Central_Air + Second_Flr_SF +
TotRms_AbvGrd +
First_Flr_SF
Df Sum of Sq RSS AIC
```

+ Street 1 1.028e+09 2.1532e+12 42677

<none>

2.1542e+12 42676

Other Criteria – BIC

Other Criteria – P-value Selection (α = 0.05)

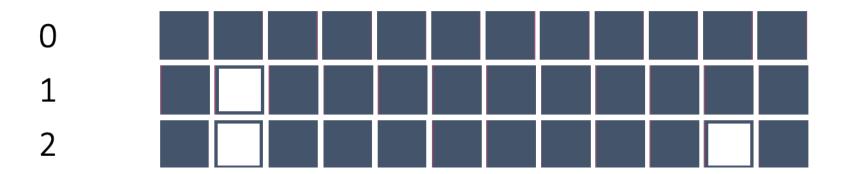
```
full.model <- lm(Sale_Price ~ ., data = train_sel)</pre>
empty.model <- lm(Sale_Price ~ 1, data = train_sel)</pre>
for.model <- step(empty.model,</pre>
                   scope = list(lower = empty.model,
                                 upper = full.model),
                   direction = "forward", k = qchisq(0.05, 1, lower.tail = FALSE))
```

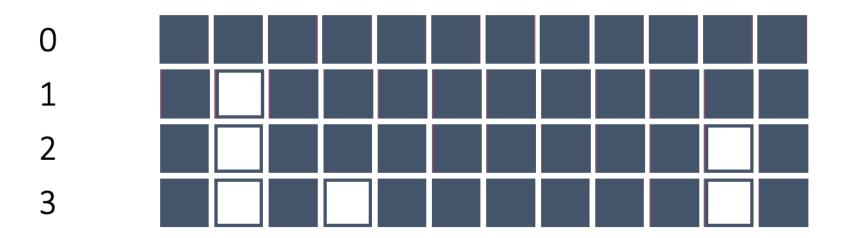
P-value selection with alpha = 0.05 Can easily change alpha to any number...

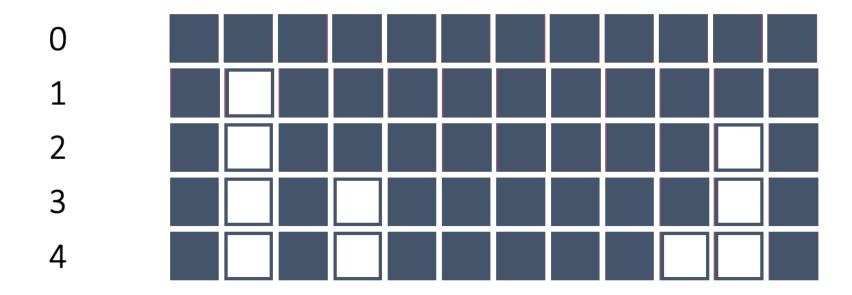
Backward Selection

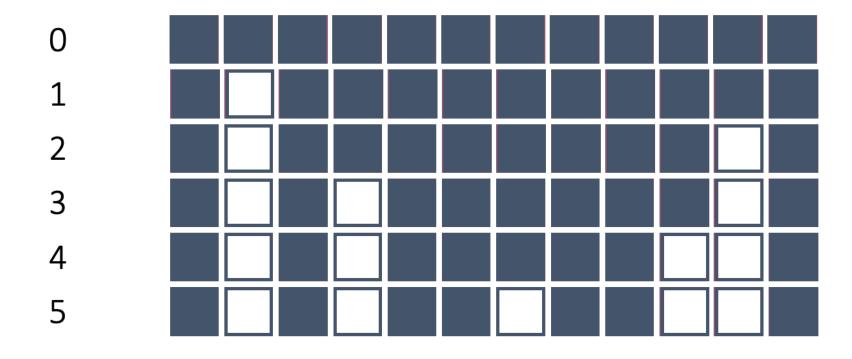
- Systematically removes variables "not informative" in the model (one variable at a time).
- 1. Start with full model with all variables (this is the base model)
- 2. Create models such that each model has exactly one predictor variable removed from it and calculate the criterion for each model
- 3. See which linear regression is best (based on criterion)
- 4. If better than base model, continue to next step... otherwise STOP (this is your model)
- 5. Update base model to this new model, repeat whole process...

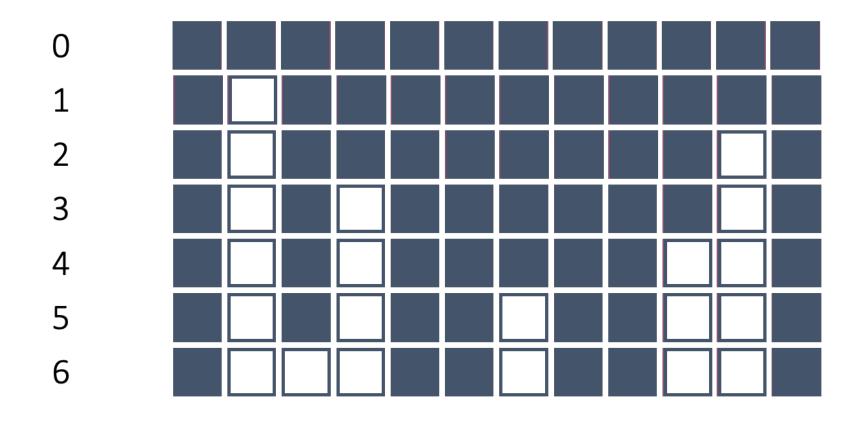


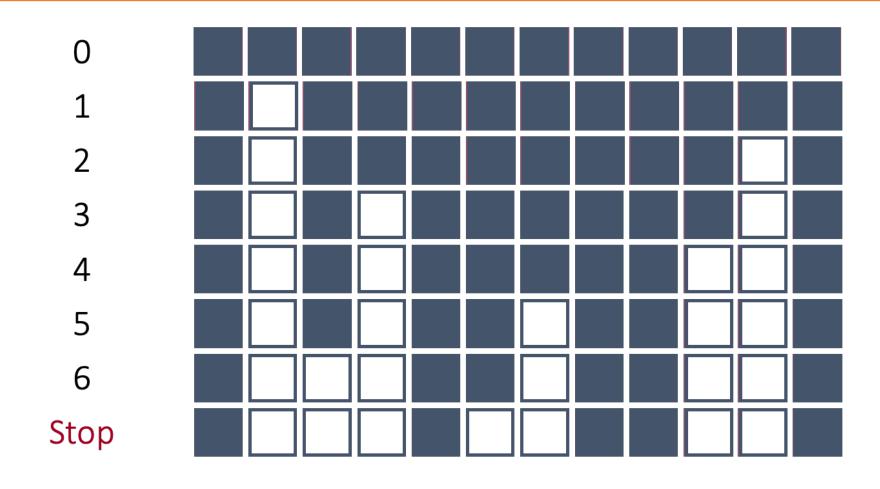












- Step 1
- AIC from base model at top of output.
- Shows the removal ("-") of each variable and the "new" AIC from that model.
- Worst variable (most likely to remove) at top.

```
Start: AIC=42677.12
Sale Price ~ Lot Area + Street + Bldg Type +
House Style + Overall Qual + Roof Style + Central Air
+ First Flr SF + Second Flr SF + Full Bath +
Half Bath + Fireplaces + Garage Area + Gr Liv Area +
TotRms AbvGrd
               Df Sum of Sq RSS
                                          AIC
                1 4.9138e+08 2.1537e+12 42676
- Gr Liv Area
- Street
                1 1.0280e+09 2.1542e+12 42676
                             2.1532e+12 42677
<none>
- First Flr SF 1 3.1548e+09 2.1563e+12 42678
- TotRms AbvGrd 1 3.4112e+09 2.1566e+12 42678
- Second Flr SF 1 6.4939e+09 2.1597e+12 42681
- Central Air
                1 1.6533e+10 2.1697e+12 42691
- Roof Style
                 5 2.8786e+10 2.1820e+12 42694
- Half Bath
                1 3.5009e+10 2.1882e+12 42708
                1 3.5997e+10 2.1892e+12 42709
- Lot Area
- Fireplaces
                1 3.6853e+10 2.1900e+12 42710
- House Style
                7 7.0980e+10 2.2241e+12 42730
- Garage_Area
                1 6.4143e+10 2.2173e+12 42735
- Bldg Type
                 4 7.1274e+10 2.2244e+12 42736
- Full Bath
                1 6.8198e+10 2.2214e+12 42739
- Overall Qual
```

9 1.7183e+12 3.8715e+12 43862

```
Step: AIC=42675.59
Sale_Price ~ Lot_Area + Street + Bldg_Type +
House_Style + Overall_Qual + Roof_Style + Central_Air
+ First_Flr_SF + Second_Flr_SF + Full_Bath +
Half Bath + Fireplaces + Garage Area + TotRms AbvGrd
```

- Step 2
- AIC from base model at top of output.
- Shows the removal ("-")
 of each variable and the
 "new" AIC from that
 model.
- Worst variable (most likely to remove) at top.
- Watch the <none>...

```
Sum of Sq
                                   RSS
                                          AIC
                1 1.0581e+09 2.1547e+12 42675
- Street
                             2.1537e+12 42676
<none>
- TotRms AbvGrd 1 3.1247e+09 2.1568e+12 42677
- Central Air
                1 1.6456e+10 2.1701e+12 42689
- Roof Style
                5 2.8773e+10 2.1824e+12 42693
- Half Bath
                1 3.5031e+10 2.1887e+12 42707
- Lot Area
                1 3.6074e+10 2.1897e+12 42708
- Fireplaces
                1 3.6944e+10 2.1906e+12 42708
- House Style
                7 7.2205e+10 2.2259e+12 42729
- Garage Area
                1 6.4018e+10 2.2177e+12 42734
- Bldg Type
                4 7.1756e+10 2.2254e+12 42735
- Full Bath
                1 6.9016e+10 2.2227e+12 42738
- Second Flr SF 1 1.2417e+11 2.2778e+12 42789
- First Flr SF
                1 1.4119e+11 2.2949e+12 42804
- Overall Qual
                9 1.7192e+12 3.8728e+12 43861
```

```
Step: AIC=42674.6
Sale_Price ~ Lot_Area + Bldg_Type + House_Style +
Overall_Qual + Roof_Style + Central_Air +
First_Flr_SF + Second_Flr_SF + Full_Bath + Half_Bath
+ Fireplaces + Garage Area + TotRms AbvGrd
```

- Step 3
- Exit the algorithm since <none> is the highest step.

```
Df Sum of Sq
                                  RSS
                                        AIC
                            2.1547e+12 42675
<none>
- TotRms AbvGrd 1 2.9784e+09 2.1577e+12 42675
- Central Air 1 1.7247e+10 2.1720e+12 42689
- Roof Style 5 2.8560e+10 2.1833e+12 42692
- Half Bath
               1 3.4751e+10 2.1895e+12 42705
- Lot Area
               1 3.5041e+10 2.1898e+12 42706
- Fireplaces 1 3.6680e+10 2.1914e+12 42707
- House_Style 7 7.3149e+10 2.2279e+12 42729
- Garage Area
                1 6.3520e+10 2.2182e+12 42732
- Bldg Type
                4 7.3044e+10 2.2278e+12 42735
- Full Bath
               1 6.8973e+10 2.2237e+12 42737
- Second Flr SF 1 1.2513e+11 2.2798e+12 42788
- First Flr SF 1 1.4221e+11 2.2969e+12 42804
- Overall Qual
               9 1.7202e+12 3.8749e+12 43860
```

Other Criteria – BIC

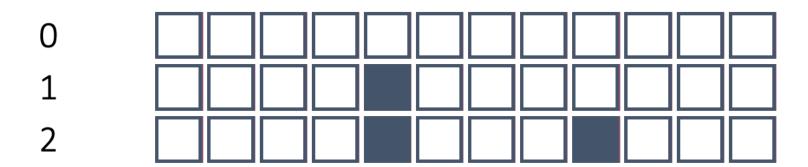
Other Criteria – P-value Selection (α = 0.05)

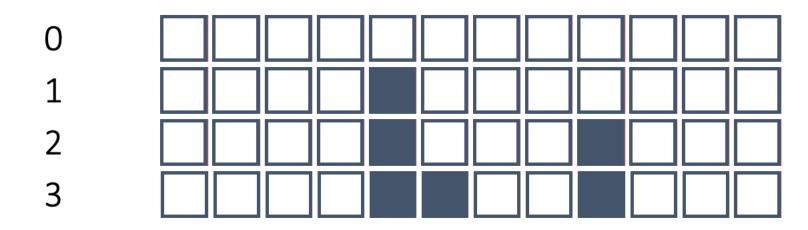
```
full.model <- lm(Sale_Price ~ ., data = train_sel)</pre>
empty.model <- lm(Sale_Price ~ 1, data = train_sel)</pre>
back.model <- step(full.model,</pre>
                   scope = list(lower = empty.model,
                                 upper = full.model),
                   direction = "backward", k = qchisq(0.05, 1, lower.tail = FALSE))
                                               P-value selection with alpha = 0.05
```

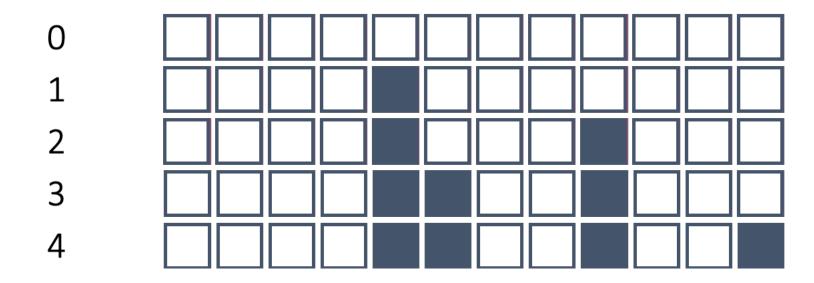
Can easily change alpha to any number...

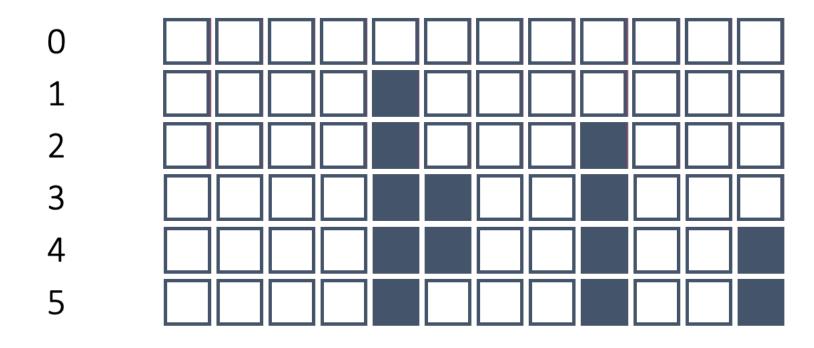
- Start with a "null" model (just the intercept) and build the model (one variable at a time), but can also **delete** variables.
- 1. Start with intercept only model (this is the base model)
- 2. For each variable not in model, create a linear regression model with the base model plus this variable
- 3. For each variable in the model, create models with the base model taking away one variable at a time
- 4. See which linear regression is best (based on criterion)
- 5. If better than base model, continue to next step... otherwise STOP (this is your model)
- 6. Update base model to this new model, repeat whole process...

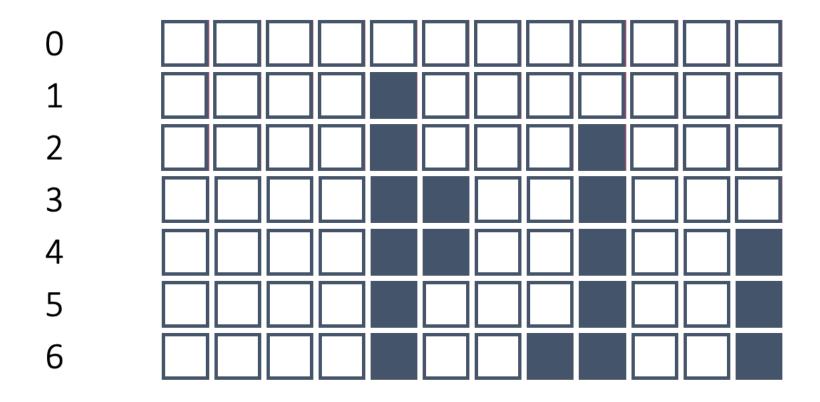


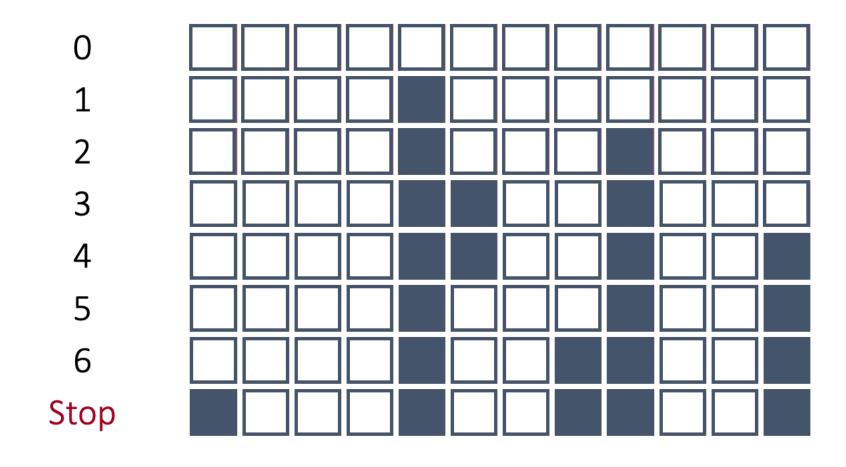












Start: AIC=46323.64 Sale Price ~ 1

- Step 1
- AIC from base model at top of output.
- Shows the addition ("+")
 of each variable and the
 "new" AIC from that
 model.
- Best variable at top.

```
Sum of Sq
                                     RSS
                Df
                                           AIC
                 9 9.3437e+12 3.8531e+12 43817
+ Overall Qual
                 1 6.4389e+12 6.7578e+12 44953
+ Gr Liv Area
                 1 5.3561e+12 7.8407e+12 45258
+ Garage Area
+ First Flr SF
                 1 4.8867e+12 8.3100e+12 45377
+ Full Bath
                 1 3.7827e+12 9.4141e+12 45633
+ TotRms AbvGrd
                 1 3.2304e+12 9.9663e+12 45750
+ Fireplaces
                 1 2.9715e+12 1.0225e+13 45802
                 1 1.1209e+12 1.2076e+13 46144
+ Half Bath
+ Roof Style
                 5 1.0724e+12 1.2124e+13 46160
+ Central Air
                 1 9.6147e+11 1.2235e+13 46170
+ House Style
                 7 1.0245e+12 1.2172e+13 46172
+ Second Flr SF
                 1 9.4611e+11 1.2251e+13 46173
+ Lot Area
                 1 9.0332e+11 1.2293e+13 46180
                 4 4.6434e+11 1.2732e+13 46258
+ Bldg Type
+ Street
                 1 3.1752e+10 1.3165e+13 46321
                              1.3197e+13 46324
<none>
```

Step: AIC=43816.66
Sale Price ~ Overall Qual

- Step 2
- AIC from base model at top of output.
- Shows the addition ("+")
 or removal ("-") of each
 variable and the "new"
 AIC from that model.
- Best choice at top.
- Watch the <none>...

```
Sum of Sq
                                     RSS
                Df
                                           AIC
                 1 9.8905e+11 2.8640e+12 43210
+ Gr Liv Area
+ First Flr SF
                 1 5.2665e+11 3.3264e+12 43517
+ Garage Area
                 1 4.6644e+11 3.3866e+12 43554
+ TotRms AbvGrd
                 1 4.6123e+11 3.3918e+12 43557
+ Full Bath
                 1 4.1206e+11 3.4410e+12 43587
+ Fireplaces
                 1 4.0551e+11 3.4476e+12 43591
+ Lot Area
                 1 3.8148e+11 3.4716e+12 43605
+ Bldg Type
                 4 2.3715e+11 3.6159e+12 43694
+ Second Flr SF
                 1 1.7555e+11 3.6775e+12 43723
+ Half Bath
                 1 1.3948e+11 3.7136e+12 43743
+ Central Air
                 1 9.1322e+10 3.7617e+12 43769
+ House Style
                 7 6.1815e+10 3.7912e+12 43797
+ Roof Style
                 5 5.1448e+10 3.8016e+12 43799
                              3.8531e+12 43817
<none>
                 1 1.9573e+06 3.8531e+12 43819
+ Street
                 9 9.3437e+12 1.3197e+13 46324
- Overall Qual
```

Step: AIC=43210.24
Sale_Price ~ Overall_Qual + Gr_Liv_Area

- Step 3
- AIC from base model at top of output.
- Shows the addition ("+")
 or removal ("-") of each
 variable and the "new"
 AIC from that model.
- Best choice at top.
- Watch the <none>...

```
Df
                   Sum of Sq
                                    RSS
                                          AIC
                 7 2.5351e+11 2.6105e+12 43034
+ House Style
                 1 2.1638e+11 2.6476e+12 43051
+ Garage Area
                 1 1.3097e+11 2.7330e+12 43116
+ Lot Area
+ First Flr SF
                 1 1.2210e+11 2.7419e+12 43123
+ Fireplaces
                 1 1.1069e+11 2.7533e+12 43131
+ Central Air
                 1 1.1050e+11 2.7535e+12 43132
+ Second Flr SF
                 1 1.0207e+11 2.7619e+12 43138
+ Bldg Type
                 4 1.0299e+11 2.7610e+12 43143
+ Roof Style
                 5 6.0726e+10 2.8033e+12 43176
                 1 3.2970e+10 2.8310e+12 43188
+ Full Bath
+ TotRms AbvGrd
                 1 2.4688e+10 2.8393e+12 43194
                             2.8640e+12 43210
<none>
                 1 4.0261e+07 2.8640e+12 43212
+ Half Bath
                 1 2.2632e+07 2.8640e+12 43212
+ Street
- Gr Liv Area
                 1 9.8905e+11 3.8531e+12 43817
                 9 3.8938e+12 6.7578e+12 44953
- Overall Qual
```

```
Step: AIC=42674.6
Sale_Price ~ Overall_Qual + House_Style +
Garage_Area + Bldg_Type + Fireplaces + Full_Bath
+ Half_Bath + Lot_Area + Roof_Style +
Central_Air + Second_Flr_SF + TotRms_AbvGrd +
First Flr SF
```

- Step 14
- Exit the algorithm since <none> is the highest step.

```
Df Sum of Sq RSS AIC
                             2.1547e+12 42675
<none>
                1 2.9784e+09 2.1577e+12 42675
- TotRms AbvGrd
+ Street
                1 1.0581e+09 2.1537e+12 42676
                1 5.2156e+08 2.1542e+12 42676
+ Gr Liv Area
- Central Air
                1 1.7247e+10 2.1720e+12 42689
- Roof Style
                5 2.8560e+10 2.1833e+12 42692
- Half Bath
                1 3.4751e+10 2.1895e+12 42705
- Lot Area
                1 3.5041e+10 2.1898e+12 42706
- Fireplaces
                1 3.6680e+10 2.1914e+12 42707
                7 7.3149e+10 2.2279e+12 42729
- House Style
- Garage Area
                1 6.3520e+10 2.2182e+12 42732
- Bldg Type
                4 7.3044e+10 2.2278e+12 42735
- Full Bath
                1 6.8973e+10 2.2237e+12 42737
- Second Flr SF
                1 1.2513e+11 2.2798e+12 42788
- First Flr SF
                1 1.4221e+11 2.2969e+12 42804
- Overall Qual
                9 1.7202e+12 3.8749e+12 43860
```

Other Criteria – BIC

Other Criteria – P-value Selection (α = 0.05)

```
full.model <- lm(Sale_Price ~ ., data = train_sel)</pre>
empty.model <- lm(Sale_Price ~ 1, data = train_sel)</pre>
step.model <- step(empty.model,</pre>
                   scope = list(lower = empty.model,
                                 upper = full.model),
                   direction = "both", k = qchisq(0.05, 1, lower.tail = FALSE))
```

P-value selection with alpha = 0.05 Can easily change alpha to any number...

Issues with Automatic Search Algorithms

- Automated model selection results in the following:
 - Biases in parameter estimates, predictions, and standard errors
 - Incorrect calculation of degrees of freedom (p-value method)
 - P-values that tend to err on the side of overestimating significance (increasing Type I Error probability)
- Can result in locally best model (not global)
- DO NOT blindly use result from automatic search algorithm as final model!!

Significance Levels

Conservative P-values (Adrian Raftery, 1994)

	Sample Size					
Evidence	30	50	100	1,000	10,000	100,000
Weak	.076	.053	.032	.009	.002	.0007
Fair	.028	.019	.010	.003	.0008	.0002
Strong	.005	.003	.001	.0003	.0001	.00003
Very Strong	.001	.0005	.0001	.00004	.00001	.000004

In Summary...

- Automatic stepwise search algorithms can help provide a subset of potential variables
- NO model chosen from one of these algorithms should be blindly selected as the final model (always explore other potential models and investigate model assumptions)
- If you use p-values for your selection, be sure to *adjust your p-values* if you have a large sample size