Model Selection

Class of 2023

Review

- Simple Linear Regression
- Multiple Linear Regression
- With many explanatory variables, how do we know which ones are most informative?

Ames Housing Data

Sale Price =

Total rooms above-ground

Second Floor SF

First Floor SF

Fireplaces

Full baths

Garage Area

Many Other Variables to Choose from

Model Building

- Information Criteria
- Selection Algorithms
  - Forward Selection
  - Backward Elimination
  - Stepwise
- Discussion of p-values

Model Building

- Should ALWAYS be done with training data!

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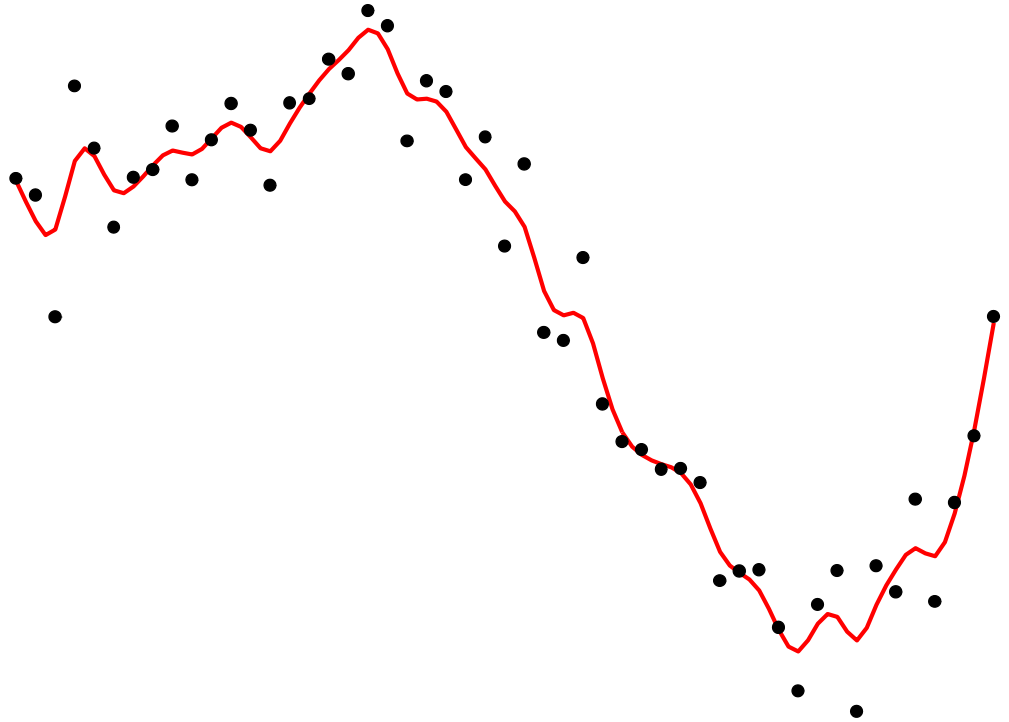
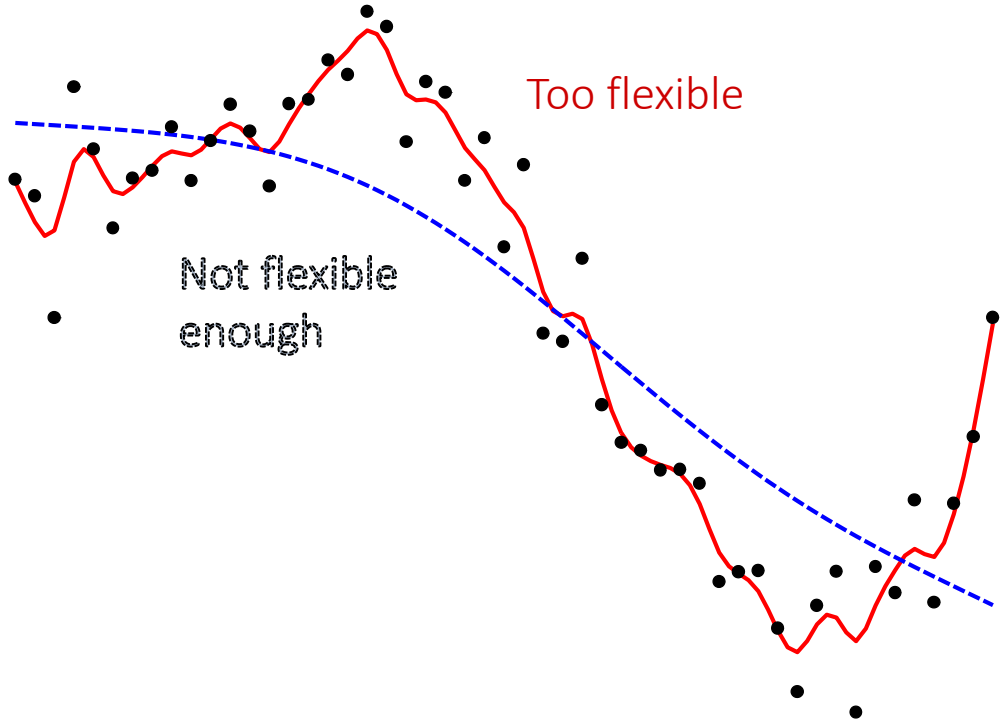


...

Model Building

- Should ALWAYS be done with training data!



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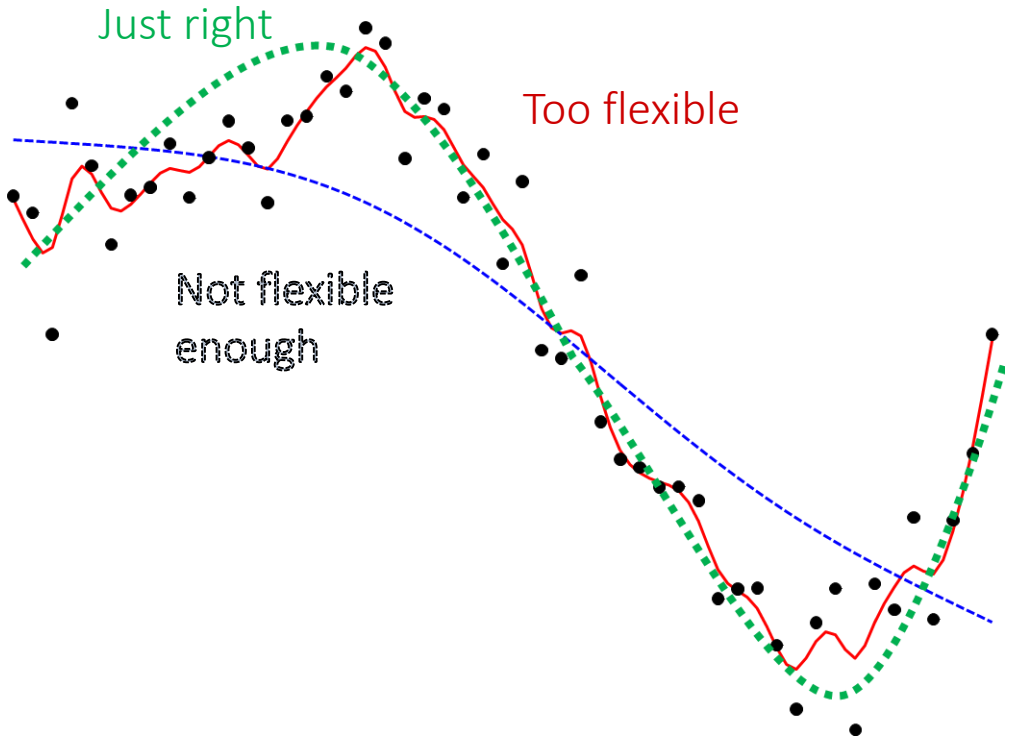
Model Building

- Should ALWAYS be done with training data!



Information Criteria

Information Criteria

- Good to compare models (no one value “cutoff”)
- Uses the likelihood of the data with some penalty
- Two of the most common Information criteria are:
  - AIC: Akaiki Information Criteria
  - BIC: Bayesian Information Criteria
- Smaller is better!!

More on Information Criteria

- Different criteria have different penalties
  - AIC penalty: 2p
  - BIC penalty: plog(n)

  Where p= # estimated parameters and n=sample size

Forward Selection

Forward Selection

In forward selection, we start with a “null” model (just the intercept) and systematically build the model (one variable at a time)

0. Start with a null model, this is the base model

1. For each variable not in model, create a linear regression model with the base model plus this variable

2. See which linear regression is best (based on criterion)

3. Is this regression better than the base model?

    a. Yes, then continue on to step 4

    b. No, exit the algorithm with the base model as the chosen model

4. The base model is now the previous base model plus the variable selected in step 3. Using this as your new base model, go back to step 1 and continue.

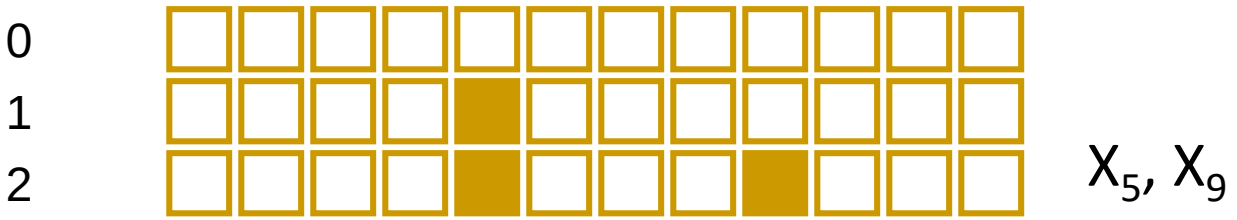
Forward Selection

0 

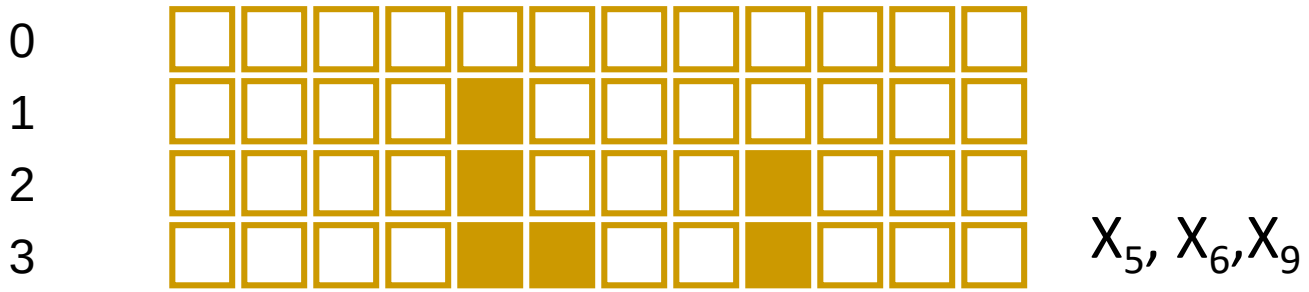
There are 12 potential variables

Forward Selection

Forward Selection

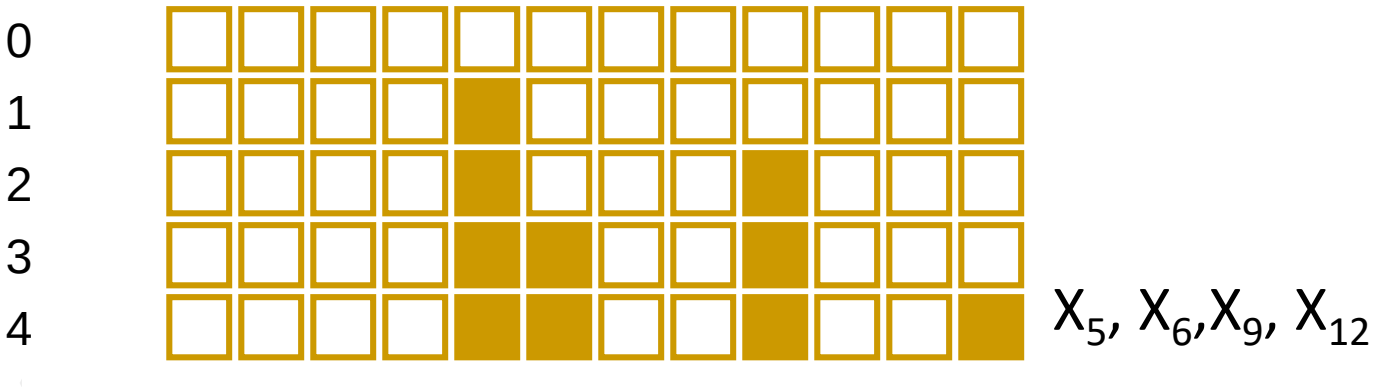


Forward Selection

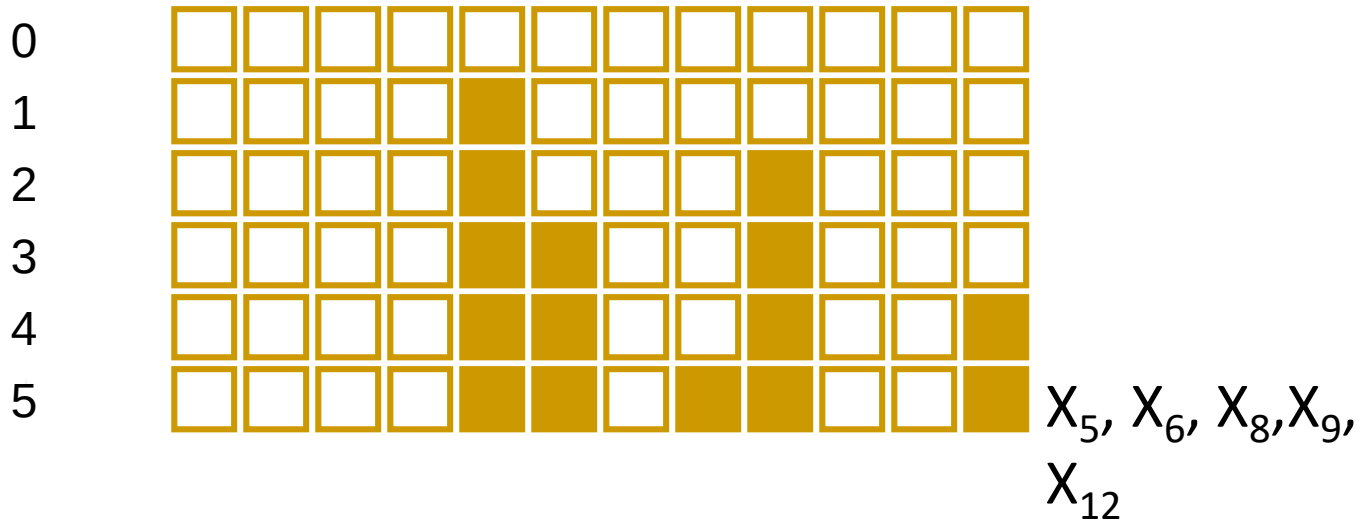


X_5, X_6,X_9

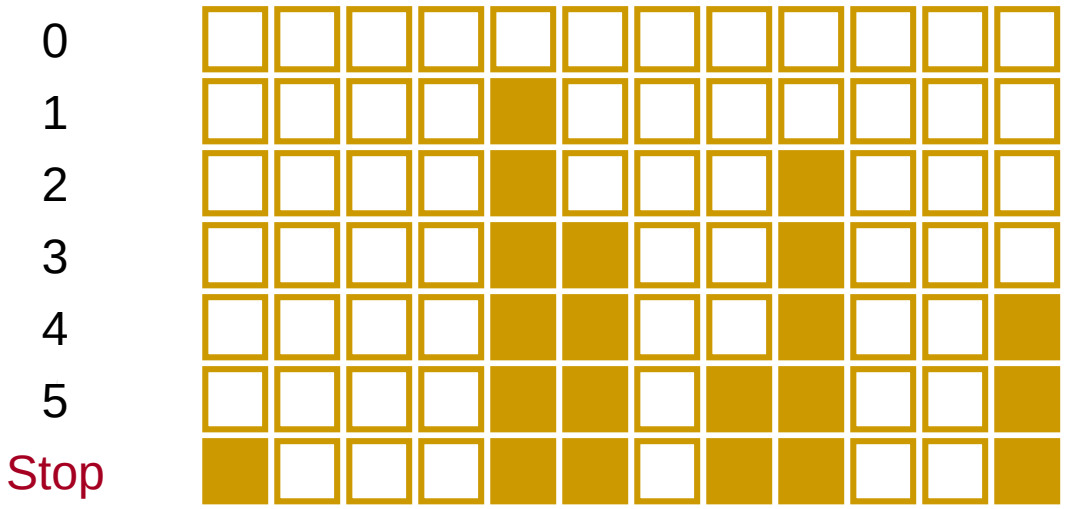
Forward Selection



Forward Selection

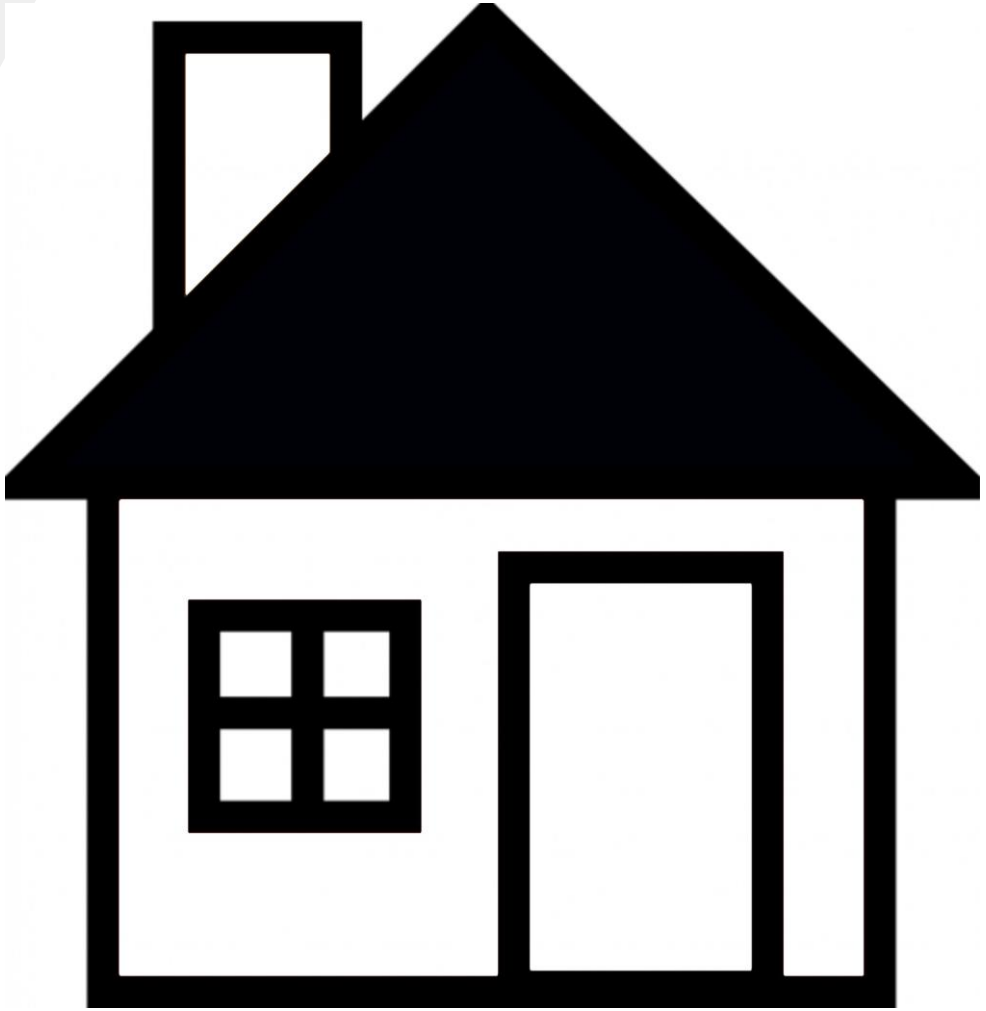


Forward Selection



Final Model includes: X_1,X_5, X_6, X_8,X_9, X_{12}

Ames Housing data



Data

```
train_sel = train %>%
  select(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`) %>%
  replace(is.na(.), 0)
```

Forward Selection Code

```
# Create full model and empty model
full.model <- lm(Sale_Price ~ . , data = train_sel)
empty.model <- lm(Sale_Price ~ 1, data = train_sel)

# k = 2 for AIC selection
for.model <- step(empty.model,
                  scope = list(lower = empty.model,
                               upper = full.model),
                  direction = "forward", k = 2)
```

Step 1

```
Start:  AIC=46323.64
Sale_Price ~ 1

                 Df  Sum of Sq         RSS   AIC
+ Overall_Qual    9 9.3437e+12 3.8531e+12 43817
+ Gr_Liv_Area     1 6.4389e+12 6.7578e+12 44953
+ Garage_Area     1 5.3561e+12 7.8407e+12 45258
+ 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
+ Bldg_Type       4 4.6434e+11 1.2732e+13 46258
+ Street          1 3.1752e+10 1.3165e+13 46321
<none>                        1.3197e+13 46324
```

Step 2

```
Step:  AIC=43816.66
Sale_Price ~ Overall_Qual

                 Df  Sum of Sq        RSS   AIC
+ Gr_Liv_Area     1 9.8905e+11 2.8640e+12 43210
+ 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
<none>                        3.8531e+12 43817
+ Street          1 1.9573e+06 3.8531e+12 43819
```

Step 3

```
Step:  AIC=43210.24
Sale_Price ~ Overall_Qual + Gr_Liv_Area

                 Df  Sum of Sq        RSS   AIC
+ House_Style     7 2.5351e+11 2.6105e+12 43034
+ Garage_Area     1 2.1638e+11 2.6476e+12 43051
+ Lot_Area        1 1.3097e+11 2.7330e+12 43116
+ 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
+ TotRms_AbvGrd   1 2.4688e+10 2.8393e+12 43194
<none>                         2.8640e+12 43210
+ Half_Bath       1 4.0261e+07 2.8640e+12 43212
+ Street          1 2.2632e+07 2.8640e+12 43212
```

Exit algorithm

```
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
<none>                  2.1542e+12 42676
+ Street  1 1.028e+09 2.1532e+12 42677
```

Other criteria

- These algorithms are referred to as stepwise because at each step, ONLY one variable can be added or taken away
- You can also use p-values as your selection criteria (penalty is a χ^2 quantile)
- Adjusted R^2 (unfortunately, R does not give you this option)

Other Criteria

```
# k = log(n) for BIC selection
for.model2 <- step(empty.model,
                   scope = list(lower = empty.model,
                                upper = full.model),
                   direction = "forward", k = log(nrow(train_sel)))

 # k = qchisq(alpha, 1, lower.tail = FALSE) for p-value with alpha selection
alpha.f=0.05
for.model3 <- step(empty.model,
                   scope = list(lower = empty.model,
                                upper = full.model),
                   direction = "forward", k = qchisq(alpha.f, 1, lower.tail = FALSE))
```

Backward Elimination

Backward Elimination

Backward elimination systematically removes variables “not informative” in the model

0. Start with full model with all predictor variables in it, this is the base model and calculate the criterion on this model

1. Create models such that each model has exactly one predictor variable removed from it and calculate the criterion for each model

2. In step 1, find the best model based on the criterion

3. Is this regression model better than the base model?

    a. Yes, then continue on to step 4

    b. No, exit the algorithm with the base model as the chosen model

4. The base model is now the model with the variable removed. Using this as your new base model, go back to step 1 and continue.

Backward Elimination

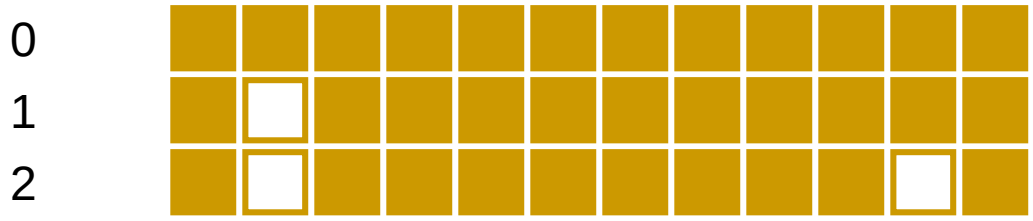
0

Start with all 12 variables in model

Backward Elimination

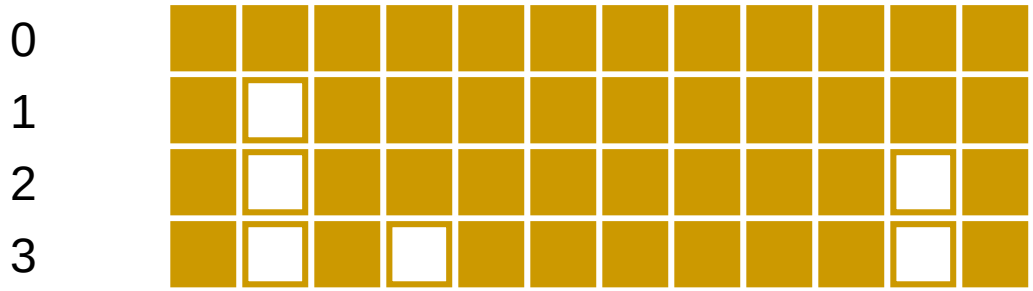
Remove x_2

Backward Elimination



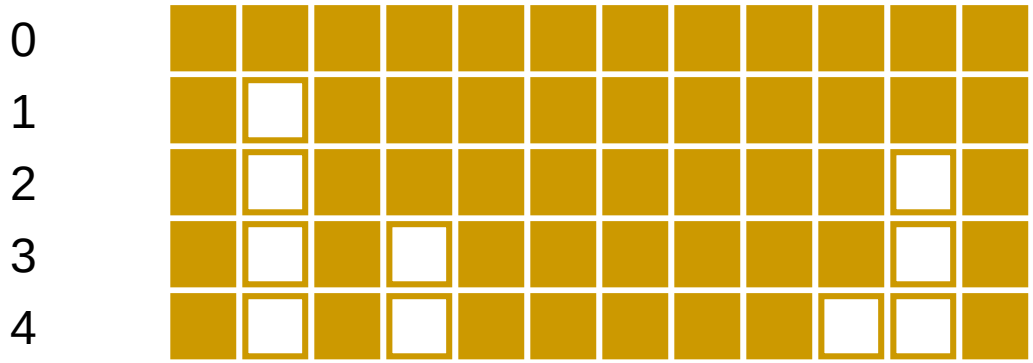
Remove x_{11}

Backward Elimination



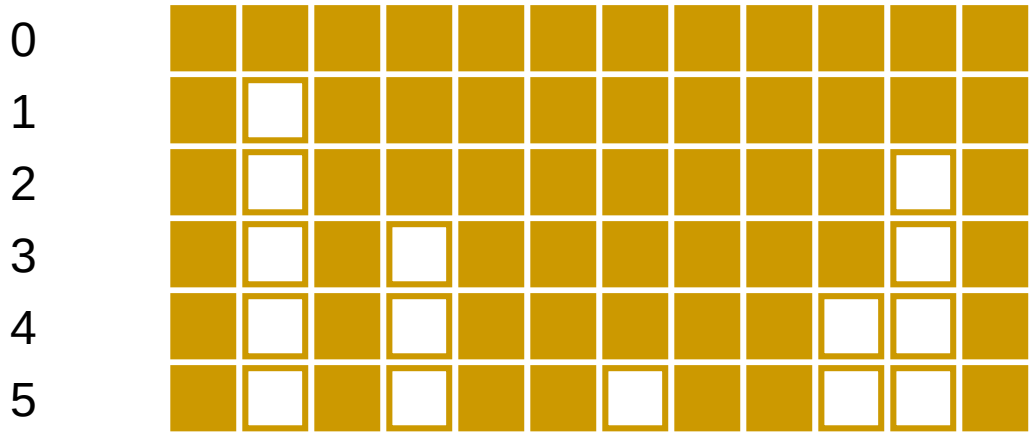
Remove x_4

Backward Elimination



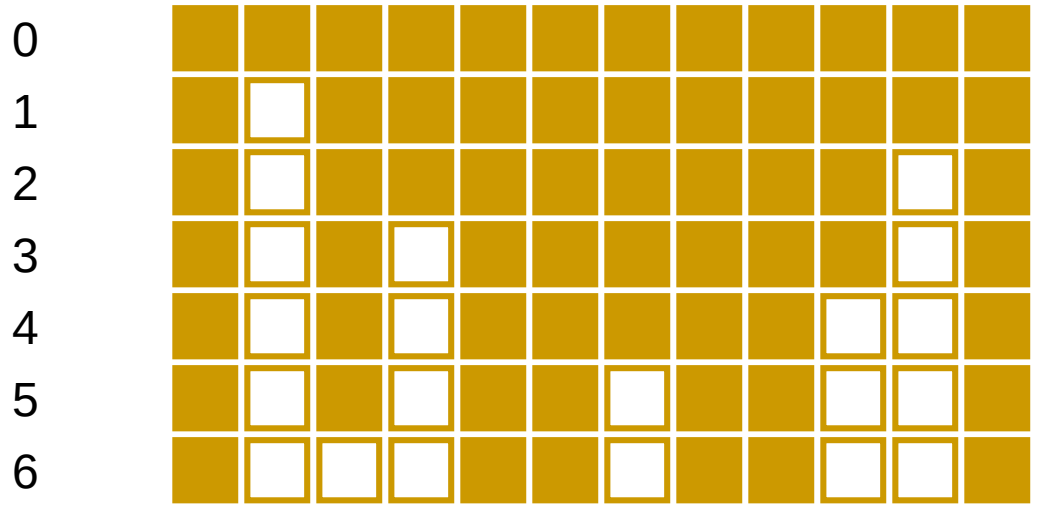
Remove x_{10}

Backward Elimination



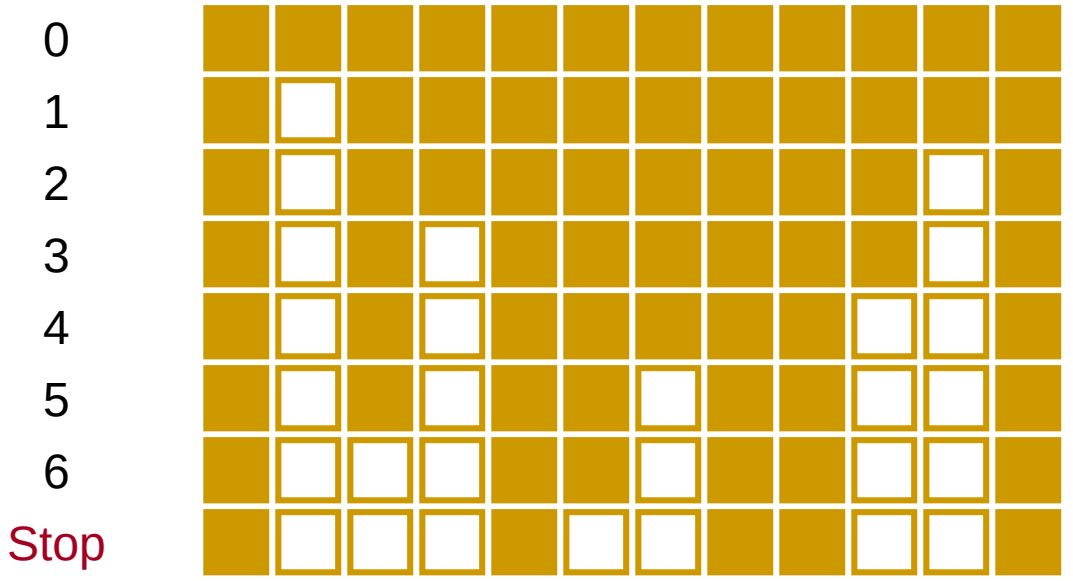
Remove x_7

Backward Elimination



Remove x_3

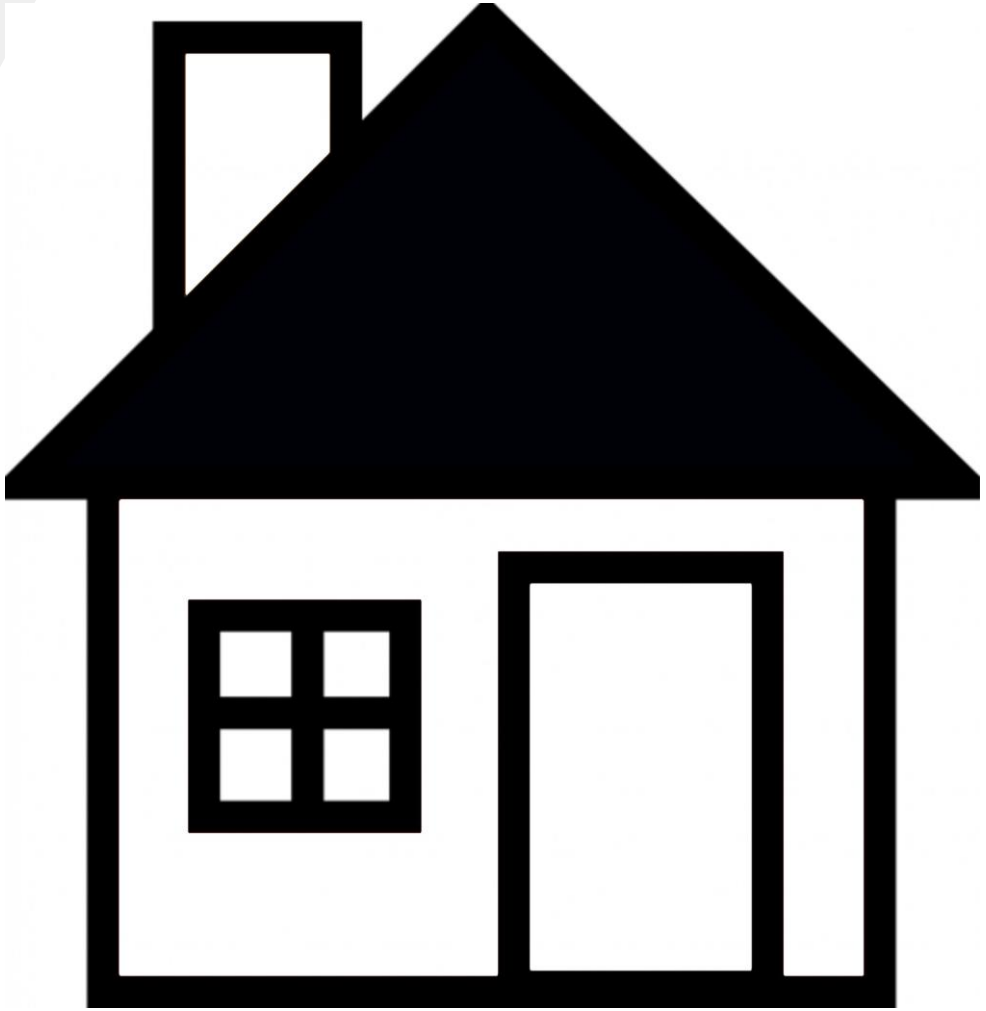
Backward Elimination



Remove x_6

Final Model includes: X_1,X_5, X_8,X_9, X_{12}

Ames Housing data



Code

```
# Create full model and empty model
full.model <- lm(Sale_Price ~ . , data = train_sel)
empty.model <- lm(Sale_Price ~ 1, data = train_sel)

# k = 2 for AIC selection
back.model <- step(full.model,
                   scope = list(lower = empty.model,
                                upper = full.model),
                   direction = "backward", k = 2)
```

Step 1

```
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
- Gr_Liv_Area    1 4.9138e+08 2.1537e+12 42676
- Street         1 1.0280e+09 2.1542e+12 42676
<none>                       2.1532e+12 42677
- 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
- Lot_Area       1 3.5997e+10 2.1892e+12 42709
- 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 2

```
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

                Df  Sum of Sq        RSS   AIC
- Street         1 1.0581e+09 2.1547e+12 42675
<none>                       2.1537e+12 42676
- 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 3 (last step)

```
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
```

	Df	Sum of Sq	RSS	AIC
<none>			2.1547e+12	42675
- 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

```
# k = log(n) for BIC selection
back.model2 <- step(full.model,
                    scope = list(lower = empty.model,
                                 upper = full.model),
                    direction = “backward", k = log(nrow(train_sel)))

# k = qchisq(alpha, 1, lower.tail = FALSE) for p-value with alpha selection
alpha.f=0.05
back.model3 <- step(full.model,
                    scope = list(lower = empty.model,
                                 upper = full.model),
                    direction = “backward", k = qchisq(alpha.f, 1, lower.tail = FALSE))
```

Stepwise selection

Stepwise Selection

Stepwise selection can systematically add or delete one variable from the model

0. Start with empty model with only the intercept in it, this is the base model and calculate the criterion on this model

1. For each variable not in model, create a linear regression model with the base model plus this variable; create additional models with the base model taking away one variable at a time

2. See which linear regression is best (based on criterion)

3. Is this regression better than the base model?

    a. Yes, then continue on to step 4

    b. No, exit the algorithm with the base model as the chosen model\

4. The base model is now the best model selected in step 3. Using this as your new base model, go back to step 1 and continue.

Stepwise selection

0 

Start with null model

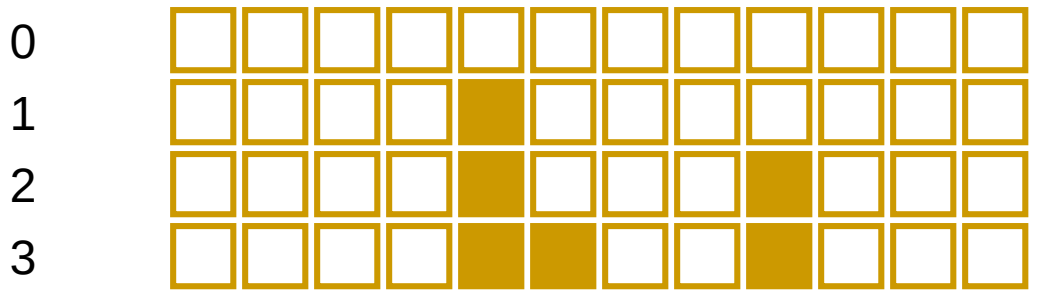
Stepwise selection

0
1

Add X_5

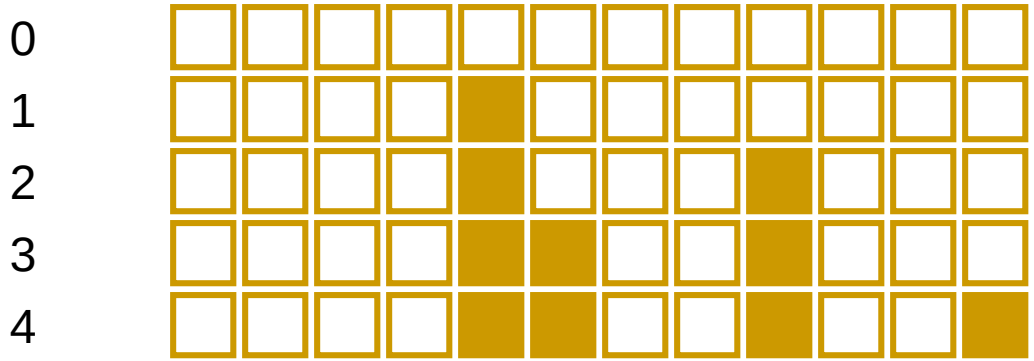
Stepwise selection

Stepwise selection



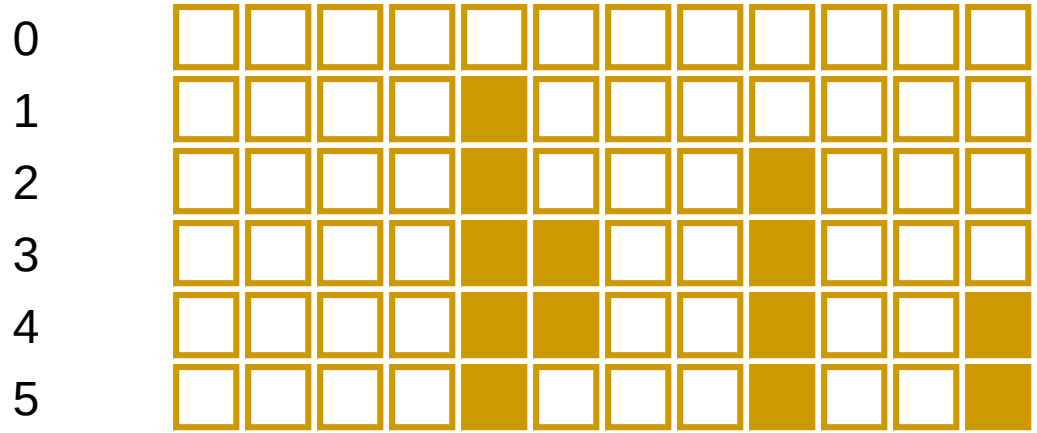
Add X_6

Stepwise selection



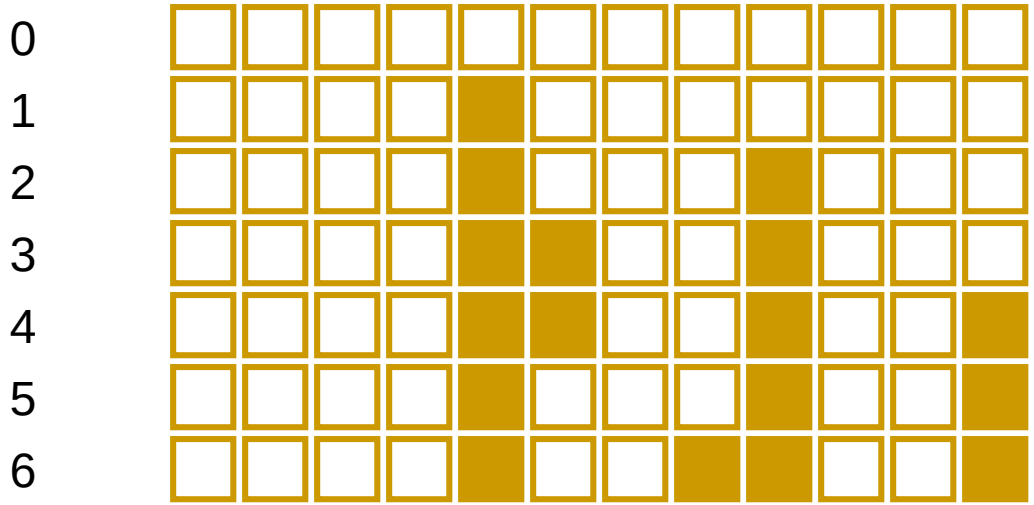
Add X_{12}

Stepwise selection



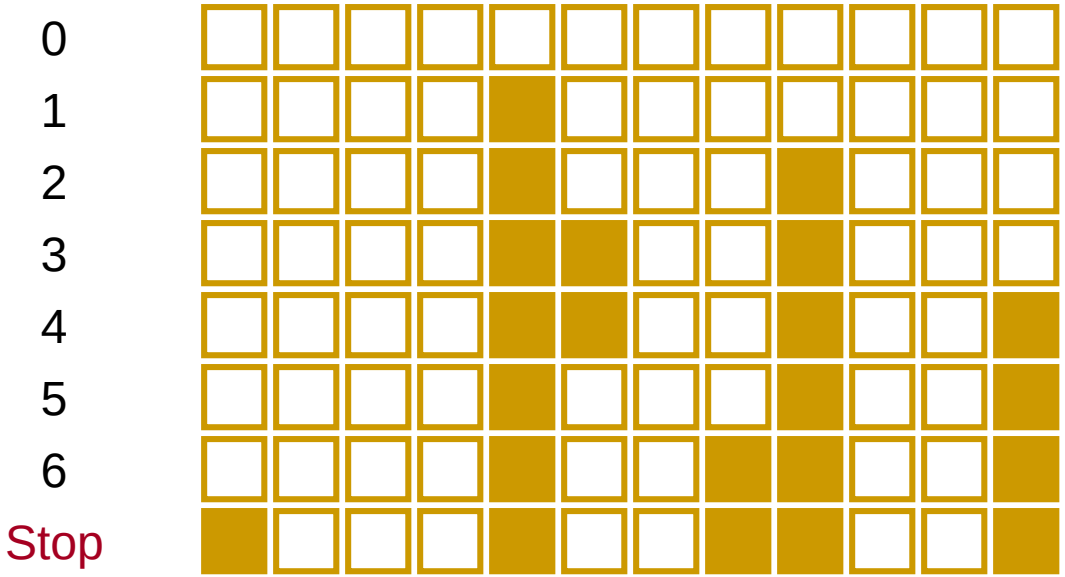
Remove X_6

Stepwise selection



Add X_8

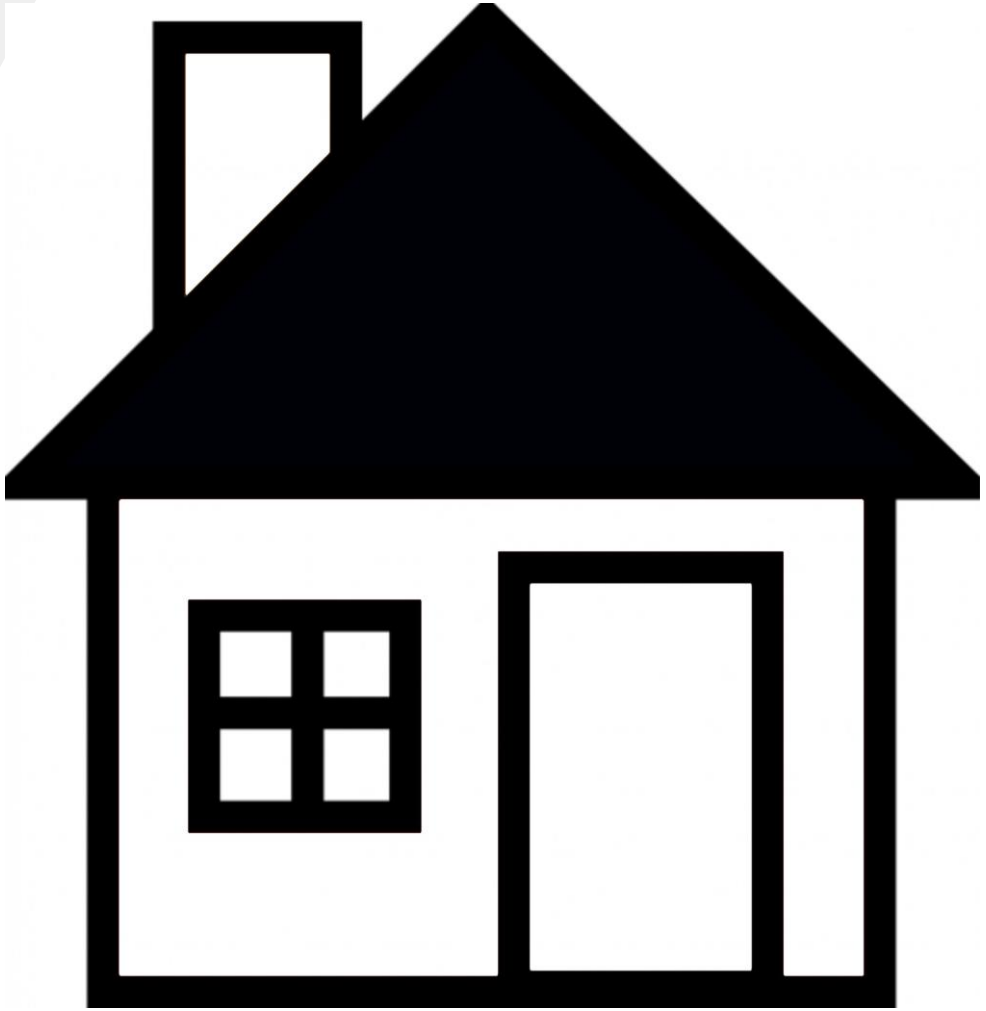
Stepwise selection



Add X_1

Final Model includes: X_1,X_5, X_8,,X_9, X_{12}

Ames Housing data



Code

```
# Create full model and empty model
full.model <- lm(Sale_Price ~ . , data = train_sel)
empty.model <- lm(Sale_Price ~ 1, data = train_sel)

# k = 2 for AIC selection
step.model <- step(empty.model,
                   scope = list(lower = empty.model,
                                upper = full.model),
                   direction = "both", k = 2)
```

Step 1

```
Start:  AIC=46323.64
Sale_Price ~ 1

                Df  Sum of Sq        RSS   AIC
+ Overall_Qual   9 9.3437e+12 3.8531e+12 43817
+ Gr_Liv_Area    1 6.4389e+12 6.7578e+12 44953
+ Garage_Area    1 5.3561e+12 7.8407e+12 45258
+ 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
+ Bldg_Type      4 4.6434e+11 1.2732e+13 46258
+ Street         1 3.1752e+10 1.3165e+13 46321
<none>                        1.3197e+13 46324
```

Step 2

```
Step:  AIC=43816.66
Sale_Price ~ Overall_Qual

                  Df  Sum of Sq        RSS   AIC
+ Gr_Liv_Area      1 9.8905e+11 2.8640e+12 43210
+ 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
<none>                         3.8531e+12 43817
+ Street           1 1.9573e+06 3.8531e+12 43819
- Overall_Qual     9 9.3437e+12 1.3197e+13 46324
```

Step 3

```
Step:  AIC=43210.24
Sale_Price ~ Overall_Qual + Gr_Liv_Area

                Df  Sum of Sq        RSS   AIC
+ House_Style    7 2.5351e+11 2.6105e+12 43034
+ Garage_Area    1 2.1638e+11 2.6476e+12 43051
+ Lot_Area       1 1.3097e+11 2.7330e+12 43116
+ 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
+ TotRms_AbvGrd  1 2.4688e+10 2.8393e+12 43194
<none>                       2.8640e+12 43210
+ Half_Bath      1 4.0261e+07 2.8640e+12 43212
+ Street         1 2.2632e+07 2.8640e+12 43212
- Gr_Liv_Area    1 9.8905e+11 3.8531e+12 43817
- Overall_Qual   9 3.8938e+12 6.7578e+12 44953
```

Exit algorithm

```
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

                Df  Sum of Sq        RSS   AIC
<none>                        2.1547e+12 42675
- TotRms_AbvGrd  1 2.9784e+09 2.1577e+12 42675
+ Street         1 1.0581e+09 2.1537e+12 42676
+ Gr_Liv_Area    1 5.2156e+08 2.1542e+12 42676
- 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

```
# k = log(n) for BIC selection
for.model2 <- step(empty.model,
                   scope = list(lower = empty.model,
                                upper = full.model),
                   direction = “both", k = log(nrow(train_sel)))

# k = qchisq(alpha, 1, lower.tail = FALSE) for p-value with alpha selection
alpha.f=0.05
for.model3 <- step(empty.model,
                   scope = list(lower = empty.model,
                                upper = full.model),
                   direction = “both", k = qchisq(alpha.f, 1, lower.tail = FALSE))
```

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

Source: Adrian Raftery, 1994

	Sample Size			
Evidence	**30**	**50**	**100**	**1000**
Weak	.076	.053	.032	.009
Fair	.028	.019	.010	.003
Strong	.005	.003	.001	.0003
Very Strong	.001	.0005	.0001	.00004

Wrap-up

- 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