cs109a_hw4

October 10, 2017

1 CS 109A/STAT 121A/AC 209A/CSCI E-109A: Homework 4

2 Regularization, High Dimensionality, PCA

Harvard University Fall 2017 Instructors: Pavlos Protopapas, Kevin Rader, Rahul Dave, Margo Levine

---

2.0.1 INSTRUCTIONS

- To submit your assignment follow the instructions given in canvas.
- Restart the kernel and run the whole notebook again before you submit.
- Do not include your name(s) in the notebook even if you are submitting as a group.
- If you submit individually and you have worked with someone, please include the name of your [one] partner below.

Your partner's name (if you submit separately):
Enrollment Status (109A, 121A, 209A, or E109A):
Import libraries:

In [12]:
```
import numpy as np
import pandas as pd
import matplotlib
import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.metrics import r2_score
from sklearn.decomposition import PCA
import statsmodels.api as sm
from statsmodels.api import OLS
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression
from sklearn.linear_model import Ridge
from sklearn.linear_model import Lasso
from sklearn.linear_model import RidgeCV
from sklearn.linear_model import LassoCV
%matplotlib inline
sns.set_context("poster")
```

3 Continuing Bike Sharing Usage Data

In this homework, we will focus on multiple linear regression, regularization, dealing with high dimensionality, and PCA. We will continue to build regression models for the Capital Bikeshare program in Washington D.C. See Homework 3 for more information about the data.

*Note: please make sure you use all the processed data from HW 3 Part (a)...you make want to save the data set on your computer and reread the csv/json file here.

In [13]:
```
# Create Dataframes
trainDf = pd.read_csv("Bikeshare_train.csv")
testDf = pd.read_csv("Bikeshare_test.csv")

# Create dummy variables
trainBinaryDf = pd.get_dummies(trainDf, columns=["season", "month", "day_of_week", "wea
testBinaryDf = pd.get_dummies(testDf, columns=["season", "month", "day_of_week", "weath

# Normalize predictors
for column in ["temp", "atemp", "humidity", "windspeed"]:
    colMean = np.mean(trainBinaryDf[column])
    colSD = np.std(trainBinaryDf[column])
    trainBinaryDf[column + "_norm"] = [(x - colMean)/float(colSD) for x in trainBinaryD
    testBinaryDf[column + "_norm"] = [(x - colMean)/float(colSD) for x in testBinaryDf[
trainBinaryDf.head()

# Drop k-th dummies
predictors = ["holiday", "workingday", "temp_norm","atemp_norm","humidity_norm","windsp
              "weather_1.0", "weather_2.0", "day_of_week_0.0", "day_of_week_1.0", "day_
              "day_of_week_3.0", "day_of_week_4.0", "day_of_week_5.0", "season_1.0",
              "season_2.0", "season_3.0", "month_2.0", "month_3.0", "month_4.0", "month
              "month_6.0", "month_7.0", "month_8.0", "month_9.0", "month_10.0", "month_

# Add a constant term to our predictors
trainBinaryDf = sm.add_constant(trainBinaryDf)
testBinaryDf = sm.add_constant(testBinaryDf)

trainPredict = trainBinaryDf[predictors]
testPredict = testBinaryDf[predictors]
```

In the above code, we simply prepared our data in the same way that we did in HW3.

3.1 Part (f): Regularization/Penalization Methods

As an alternative to selecting a subset of predictors and fitting a regression model on the subset, one can fit a linear regression model on all predictors, but shrink or regularize the coefficient estimates to make sure that the model does not "overfit" the training set.

Use the following regularization techniques to fit linear models to the training set: - Ridge regression - Lasso regression

You may choose the shrikage parameter λ from the set $\{10^{-5}, 10^{-4}, ..., 10^{4}, 10^{5}\}$ using cross-validation. In each case,

- How do the estimated coefficients compare to or differ from the coefficients estimated by a plain linear regression (without shrikage penalty) in Part (b) fropm HW 3? Is there a difference between coefficients estimated by the two shrinkage methods? If so, give an explantion for the difference.
- List the predictors that are assigned a coefficient value close to 0 (say < 1e-10) by the two methods. How closely do these predictors match the redundant predictors (if any) identified in Part (c) from HW 3?
- Is there a difference in the way Ridge and Lasso regression assign coefficients to the predictors `temp` and `atemp`? If so, explain the reason for the difference.

We next analyze the performance of the two shrinkage methods for different training sample sizes: - Generate random samples of sizes 100, 150, ..., 400 from the training set. You may use the following code to draw a random sample of a specified size from the training set:

In [14]:
```
#--------  sample
# A function to select a random sample of size k from the training set
# Input:
#      x (n x d array of predictors in training data)
#      y (n x 1 array of response variable vals in training data)
#      k (size of sample)
# Return:
#      chosen sample of predictors and responses

def sample(x, y, k):
    n = x.shape[0] # No. of training points

    # Choose random indices of size 'k'
    subset_ind = np.random.choice(np.arange(n), k)

    # Get predictors and reponses with the indices
    x_subset = x[subset_ind, :]
    y_subset = y[subset_ind]

    return (x_subset, y_subset)
```

In [ ]:

- Fit linear, Ridge and Lasso regression models to each of the generated sample. In each case, compute the R^2 score for the model on the training sample on which it was fitted, and on the test set.
- Repeat the above experiment for 10 random trials/splits, and compute the average train and test R^2 across the trials for each training sample size. Also, compute the standard deviation (SD) in each case.
- Make a plot of the mean training R^2 scores for the linear, Ridge and Lasso regression methods as a function of the training sample size. Also, show a confidence interval for the mean scores extending from **mean - SD** to **mean + SD**. Make a similar plot for the test R^2 scores.

How do the training and test R^2 scores compare for the three methods? Give an explanation for your observations. How do the confidence intervals for the estimated R^2 change with training sample size? Based on the plots, which of the three methods would you recommend when one needs to fit a regression model using a small training sample?

Hint: You may use sklearn's RidgeCV and LassoCV classes to implement Ridge and Lasso regression. These classes automatically perform cross-validation to tune the parameter λ from a given range of values. You may use the plt.errorbar function to plot confidence bars for the average R^2 scores.

In [15]:
```
# Lambdas
lambdas = [10**x for x in range(-5, 6)]
xTrain = trainPredict
yTrain = trainBinaryDf["count"]

ridgeCoefs = []
lassoCoefs = []

# Regression on entire training data set
ridge = RidgeCV(alphas=lambdas, cv=10, fit_intercept=True)
ridge.fit(xTrain, yTrain)

ridgeCoefs = ridge.coef_

lasso = LassoCV(alphas=lambdas, cv=10, max_iter=10000, fit_intercept=True)
lasso.fit(xTrain, yTrain)

lassoCoefs = lasso.coef_
```

In [16]:
```
HW3Model = sm.OLS(yTrain, xTrain).fit()
HW3Coefs = HW3Model.params
```

In [17]:
```
r2TrainVals = pd.DataFrame(data={"Original": [.576], "Lasso": [lasso.score(xTrain, yTra
                                 "Ridge": [ridge.score(xTrain, yTrain)]})
r2TrainVals
```

Out[17]:

	Lasso	Original	Ridge
0	0.563605	0.576	0.559563

In [18]:
```
xTest = testPredict
yTest = testBinaryDf["count"]
```

In [19]:
```
r2TestVals = pd.DataFrame(data={"Original": [.249], "Lasso": [lasso.score(xTest, yTest)
                                 "Ridge": [ridge.score(xTest, yTest)]})
r2TestVals
```

Out[19]:

	Lasso	Original	Ridge
0	0.263547	0.249	0.256219

In [20]:
```
ridgeCoefs[-1] = ridge.intercept_
lassoCoefs[-1] = lasso.intercept_
coefsTable = pd.DataFrame(data={"HW3Model": HW3Coefs, "RidgeModel": ridgeCoefs, "LassoM
coefsTable.head(50)
```

Out[20]:

	HW3Model	LassoModel	RidgeModel
holiday	-616.602710	-171.307907	-235.657032
workingday	-24.093294	0.000000	28.943832
temp_norm	924.334403	615.501808	596.419466
atemp_norm	311.961760	473.093575	531.323759
humidity_norm	-547.663783	-556.194283	-558.385010
windspeed_norm	-254.736916	-246.996085	-264.834036
weather_1.0	1581.978284	759.077243	480.235213
weather_2.0	1565.411700	731.541784	452.456290
day_of_week_0.0	-465.145010	-293.747624	-268.575304
day_of_week_1.0	-256.650051	-204.727796	-203.553159
day_of_week_2.0	-328.184507	-141.402923	-169.398103
day_of_week_3.0	37.612773	2.027548	67.202563
day_of_week_4.0	-71.642544	-0.000000	15.123090
day_of_week_5.0	-21.831675	19.958391	83.912409
season_1.0	-1226.186543	-980.105861	-831.421968
season_2.0	-327.357503	-0.000000	-71.167428
season_3.0	-193.304968	-225.728921	-236.541870
month_2.0	88.940093	0.000000	-43.283473
month_3.0	239.180898	21.848502	96.419673
month_4.0	333.349086	105.307226	243.948855
month_5.0	-65.812500	-0.000000	57.943527
month_6.0	-792.262899	-409.762166	-357.529453
month_7.0	-1279.987006	-633.987086	-578.242146
month_8.0	-776.475490	-79.491851	-151.051370
month_9.0	405.144566	743.960587	640.829392
month_10.0	486.250904	673.115269	607.588625
month_11.0	112.681645	114.448501	192.866358
month_12.0	-118.835819	-0.000000	-60.494888
const	3791.129801	4189.010483	4401.735647

In [21]:

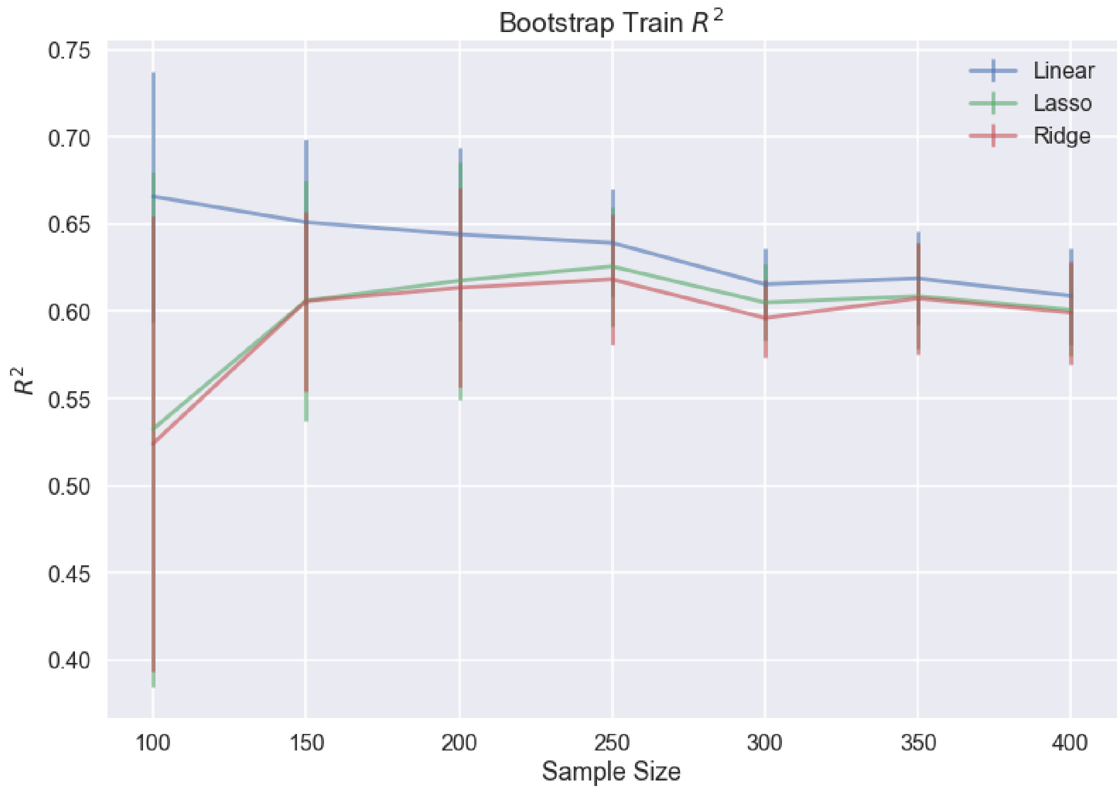
```
def randSampleR2(k):
    """k is the sample size
    outputs R2 values for linear, lasso, ridge regression models"""

    xSub, ySub = sample(xTrain.as_matrix(), yTrain.as_matrix(), k)

    ridge = RidgeCV(alphas=lambdas, cv=10, fit_intercept=True)
    ridge.fit(xSub, ySub)

    lasso = LassoCV(alphas=lambdas, cv=10, fit_intercept=True, max_iter=10000)
    lasso.fit(xSub, ySub)

    linear = sm.OLS(ySub, xSub).fit()

    yHat = linear.predict(xTest)
```

```
            return linear.rsquared, lasso.score(xSub, ySub), ridge.score(xSub, ySub), \
                   r2_score(yTest, yHat), lasso.score(xTest, yTest), ridge.score(xTest, yTest)
```

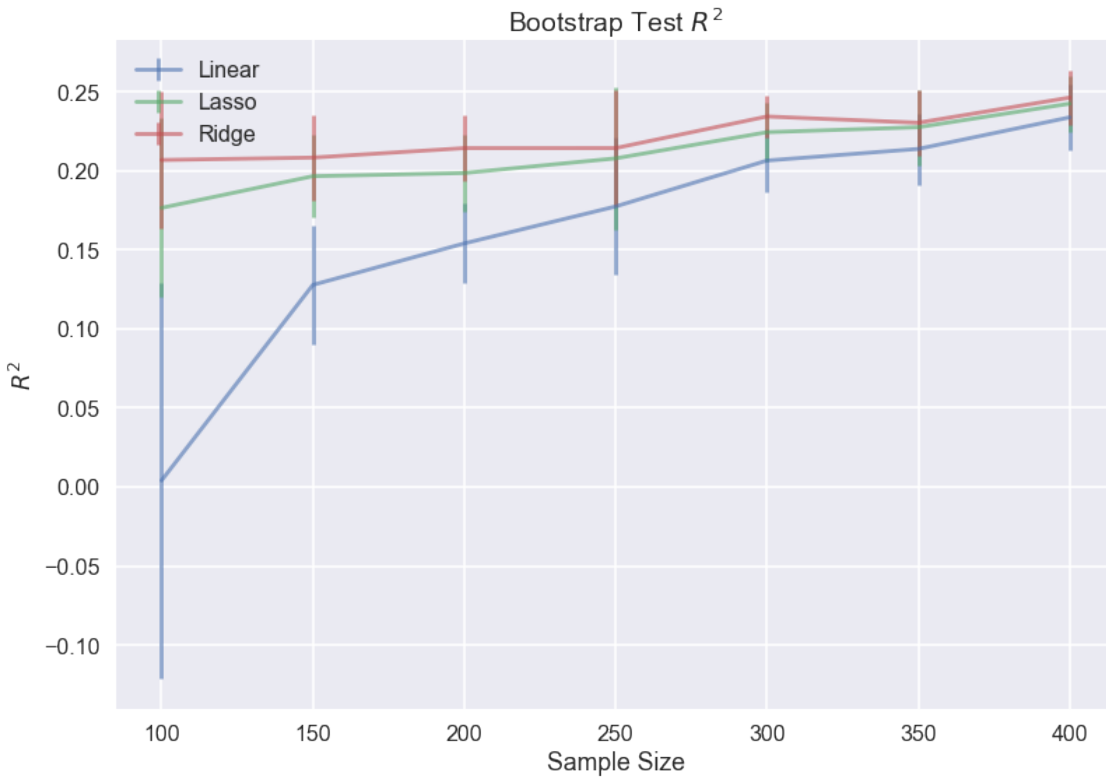
In [22]:
```
sampleSizes = np.arange(100, 450, 50)

rSquaredBootStrap = {"sampleSize": sampleSizes, "linearTrain": [], "lassoTrain": [],
                     "ridgeTrain": [], "linearTest": [], "lassoTest": [], "ridgeTest":
for k in sampleSizes:
    linearTestR2 = []
    lassoTestR2 = []
    ridgeTestR2 = []
    linearTrainR2 = []
    lassoTrainR2 = []
    ridgeTrainR2 = []
    for _ in range(10):
        linTrain, lasTrain, ridTrain, linTest, lasTest, ridTest = randSampleR2(k)
        linearTrainR2.append(linTrain)
        lassoTrainR2.append(lasTrain)
        ridgeTrainR2.append(ridTrain)
        linearTestR2.append(linTest)
        lassoTestR2.append(lasTest)
        ridgeTestR2.append(ridTest)

    rSquaredBootStrap["linearTrain"].append(linearTrainR2)
    rSquaredBootStrap["lassoTrain"].append(lassoTrainR2)
    rSquaredBootStrap["ridgeTrain"].append(ridgeTrainR2)
    rSquaredBootStrap["linearTest"].append(linearTestR2)
    rSquaredBootStrap["lassoTest"].append(lassoTestR2)
    rSquaredBootStrap["ridgeTest"].append(ridgeTestR2)
```

In [23]:
```
fig, ax = plt.subplots()

linTrainMeans = [np.mean(x) for x in rSquaredBootStrap["linearTrain"]]
linTrainSDs = [np.std(x) for x in rSquaredBootStrap["linearTrain"]]
lasTrainMeans = [np.mean(x) for x in rSquaredBootStrap["lassoTrain"]]
lasTrainSDs = [np.std(x) for x in rSquaredBootStrap["lassoTrain"]]
ridTrainMeans = [np.mean(x) for x in rSquaredBootStrap["ridgeTrain"]]
ridTrainSDs = [np.std(x) for x in rSquaredBootStrap["ridgeTrain"]]

ax.set_title("Bootstrap Train $R^2$")
ax.set_xlabel("Sample Size")
ax.set_ylabel("$R^2$")

ax.errorbar(rSquaredBootStrap["sampleSize"], linTrainMeans, linTrainSDs, label="Linear"
ax.errorbar(rSquaredBootStrap["sampleSize"], lasTrainMeans, lasTrainSDs, label="Lasso",
ax.errorbar(rSquaredBootStrap["sampleSize"], ridTrainMeans, ridTrainSDs, label="Ridge",
ax.legend()
```

Out[23]:
```
<matplotlib.legend.Legend at 0x122fb93c8>
```




```
In [24]: fig, ax = plt.subplots()

         linTestMeans = [np.mean(x) for x in rSquaredBootStrap["linearTest"]]
         linTestSDs = [np.std(x) for x in rSquaredBootStrap["linearTest"]]
         lasTestMeans = [np.mean(x) for x in rSquaredBootStrap["lassoTest"]]
         lasTestSDs = [np.std(x) for x in rSquaredBootStrap["lassoTest"]]
         ridTestMeans = [np.mean(x) for x in rSquaredBootStrap["ridgeTest"]]
         ridTestSDs = [np.std(x) for x in rSquaredBootStrap["ridgeTest"]]

         ax.set_title("Bootstrap Test $R^2$")
         ax.set_xlabel("Sample Size")
         ax.set_ylabel("$R^2$")

         ax.errorbar(rSquaredBootStrap["sampleSize"], linTestMeans, linTestSDs, label="Linear", 
         ax.errorbar(rSquaredBootStrap["sampleSize"], lasTestMeans, lasTestSDs, label="Lasso", a
         ax.errorbar(rSquaredBootStrap["sampleSize"], ridTestMeans, ridTestSDs, label="Ridge", a
         ax.legend()

Out[24]: <matplotlib.legend.Legend at 0x1232bae10>
```



3.2 Response to above questions

- How do the estimated coefficients compare to or differ from the coefficients estimated by a plain linear regression (without shrikage penalty) in Part (b) fropm HW 3? Is there a difference between coefficients estimated by the two shrinkage methods? If so, give an explantion for the difference.

As we can see from the data table above, the magnitude of our Lasso and Ridge coefficients are significantly and consistently smaller than those of our HW3 model. This is exactly the behavior we would expect, as Lasso and Ridge methods try to decrease the magnitude of our coefficients by adding a cost term for the L1 or L2 of our β.

- List the predictors that are assigned a coefficient value close to 0 (say < 1e-10) by the two methods. How closely do these predictors match the redundant predictors (if any) identified in Part (c) from HW 3?

Lasso Model: *working_day*, *day_of_week_4.0*, *season_2.0*, *month_2.0*, *month_5.0*, *month_12.0*. We note that there are no coefficient values close to 0 in either Ridge or our HW3 models. This makes sense, as shown in class, that it is more likely for the L1 norm cost function to result in coefficients of value 0 than for L2 norm.

- Is there a difference in the way Ridge and Lasso regression assign coefficients to the predictors `temp` and `atemp`? If so, explain the reason for the difference.

Both Ridge and Lasso regression preserves the initial relationship observed in HW3, that *temp* has a larger coefficient value than *atemp*. However, what is interesting to note is that the difference between these coefficients seem to converge to 0 as our cost term increases its L^i dimensional norm. For example, for Lasso in L1, the difference is much larger than for Ridge, which uses L^2.

- How do the training and test R^2 scores compare for the three methods? Give an explanation for your observations. How do the confidence intervals for the estimated R^2 change with training sample size? Based on the plots, which of the three methods would you recommend when one needs to fit a regression model using a small training sample?

We notice that the training R^2 values for both Lasso and Ridge are lower than our HW3 model, which is to be expected as we are introducing a regularization parameter. However, our Lasso and Ridge models perform better on the test data than our HW3 model, implying that we have successfully mitigated some of the overfitting from our HW3 model.

The confidence intervals for the estimated R^2 tend to decrease as our sample size grows. While there are some fluctuations in the above graphs, we note that this overall trend of decreasing confidence intervals seems to dominate over all three models.

If we had to choose one of the three models given a small training sample, we would select the Ridge regression model. It has the smallest standard deviation in its R^2 scores, and consistently outperforms the other two models over many small sample sizes.

3.3 Part (g): Polynomial & Interaction Terms

Moving beyond linear models, we will now try to improve the performance of the regression model in Part (b) from HW 3 by including higher-order polynomial and interaction terms.

- For each continuous predictor X_j, include additional polynomial terms X_j^2, X_j^3, and X_j^4, and fit a multiple regression model to the expanded training set. How does the R^2 of this model on the test set compare with that of the linear model fitted in Part (b) from HW 3? Using a t-test, find out which of estimated coefficients for the polynomial terms are statistically significant at a significance level of 5%.
- Fit a multiple linear regression model with additional interaction terms $\mathbb{I}_{month=12} \times temp$ and $\mathbb{I}_{workingday=1} \times \mathbb{I}_{weathersit=1}$ and report the test R^2 for the fitted model. How does this compare with the R^2 obtained using linear model in Part (b) from HW 3? Are the estimated coefficients for the interaction terms statistically significant at a significance level of 5%?

In [25]:
```
# Generate polynomial features
multTrainPredict = trainPredict.copy()
multTestPredict = testPredict.copy()

for i in range(2,5):
    for var in ["temp_norm", "atemp_norm", "humidity_norm", "windspeed_norm"]:
        multTrainPredict["{}_{}".format(var, i)] = multTrainPredict[var]**i
        multTestPredict["{}_{}".format(var, i)] = multTestPredict[var]**i
```

In [26]:
```
# Fit OLS model
multModel = sm.OLS(yTrain, multTrainPredict).fit()
multModel.summary()
```

Out[26]:
```
<class 'statsmodels.iolib.summary.Summary'>
"""
                            OLS Regression Results
==============================================================================
Dep. Variable:                  count   R-squared:                       0.670
Model:                            OLS   Adj. R-squared:                  0.625
Method:                 Least Squares   F-statistic:                     15.13
Date:                Tue, 10 Oct 2017   Prob (F-statistic):           7.98e-50
Time:                        13:29:19   Log-Likelihood:                -2790.9
No. Observations:                 331   AIC:                             5662.
Df Residuals:                     291   BIC:                             5814.
Df Model:                          39
Covariance Type:            nonrobust
====================================================================================
                       coef    std err          t      P>|t|      [0.025      0.975]
------------------------------------------------------------------------------------
holiday           -526.2557    372.773     -1.412      0.159   -1259.929     207.418
workingday          14.7858    159.059      0.093      0.926    -298.265     327.837
temp_norm          770.3204    758.967      1.015      0.311    -723.441    2264.082
atemp_norm         895.9192    712.094      1.258      0.209    -505.588    2297.426
humidity_norm     -667.9033    157.118     -4.251      0.000    -977.136    -358.671
windspeed_norm    -445.8335    148.704     -2.998      0.003    -738.505    -153.162
weather_1.0       1043.9997    546.051      1.912      0.057     -30.710    2118.709
weather_2.0       1103.0116    499.023      2.210      0.028     120.859    2085.164
day_of_week_0.0   -471.0834    246.557     -1.911      0.057    -956.345      14.178
day_of_week_1.0   -227.9217    157.372     -1.448      0.149    -537.653      81.809
day_of_week_2.0   -268.0232    186.488     -1.437      0.152    -635.060      99.014
day_of_week_3.0     13.1360    196.966      0.067      0.947    -374.522     400.794
day_of_week_4.0   -104.0028    189.352     -0.549      0.583    -476.675     268.669
day_of_week_5.0     75.3419    184.193      0.409      0.683    -287.178     437.861
season_1.0       -1523.2288    467.580     -3.258      0.001   -2443.496    -602.961
season_2.0        -756.7981    536.808     -1.410      0.160   -1813.316     299.720
season_3.0          55.5255    419.974      0.132      0.895    -771.046     882.097
month_2.0         -325.0686    409.611     -0.794      0.428   -1131.245     481.108
month_3.0         -304.8491    446.028     -0.683      0.495   -1182.700     573.002
month_4.0         -418.0245    639.524     -0.654      0.514   -1676.703     840.654
month_5.0        -1037.2042    677.186     -1.532      0.127   -2370.008     295.599
month_6.0        -1456.1857    697.520     -2.088      0.038   -2829.010     -83.362
month_7.0        -1416.9882    749.751     -1.890      0.060   -2892.610      58.634
month_8.0        -1715.9389    743.240     -2.309      0.022   -3178.747    -253.131
month_9.0        -1073.4008    660.859     -1.624      0.105   -2374.069     227.268
month_10.0        -925.8710    617.522     -1.499      0.135   -2141.247     289.505
month_11.0        -825.5328    591.138     -1.397      0.164   -1988.981     337.916
month_12.0        -555.6676    479.543     -1.159      0.248   -1499.481     388.146
const             5985.5838    836.335      7.157      0.000    4339.552    7631.616
temp_norm_2      -1805.5466    814.442     -2.217      0.027   -3408.491    -202.602
atemp_norm_2      1171.9491    786.481      1.490      0.137    -375.962    2719.861
humidity_norm_2    -53.5087    154.914     -0.345      0.730    -358.402     251.384
```

```
windspeed_norm_2   -34.0621     126.569     -0.269      0.788    -283.168     215.044
temp_norm_3          8.5688     274.482      0.031      0.975    -531.653     548.790
atemp_norm_3      -302.5595     244.983     -1.235      0.218    -784.722     179.603
humidity_norm_3    -15.9849      44.689     -0.358      0.721    -103.940      71.970
windspeed_norm_3    44.6309      65.163      0.685      0.494     -83.619     172.881
temp_norm_4        -44.9184     170.385     -0.264      0.792    -380.261     290.425
atemp_norm_4       -20.6433     146.714     -0.141      0.888    -309.398     268.112
humidity_norm_4    -24.6869      31.291     -0.789      0.431     -86.272      36.898
windspeed_norm_4   -20.0552      30.144     -0.665      0.506     -79.382      39.272
==============================================================================
Omnibus:                       29.995   Durbin-Watson:                   1.959
Prob(Omnibus):                  0.000   Jarque-Bera (JB):               10.202
Skew:                          -0.094   Prob(JB):                      0.00609
Kurtosis:                       2.161   Cond. No.                     3.54e+16
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specif
[2] The smallest eigenvalue is 3.1e-29. This might indicate that there are
strong multicollinearity problems or that the design matrix is singular.
"""
```

In [27]:
```
yHatTest = multModel.predict(multTestPredict)
r2_score(yTest, yHatTest)
```

Out[27]: 0.27723843508616397

In [28]:
```
# Generate additional interaction features
intTrainPredict = multTrainPredict.copy()
intTestPredict = multTestPredict.copy()

# Add month=12 x temp interaction terms
intTrainPredict["month_12xtemp_norm"] = intTrainPredict["month_12.0"] * intTrainPredict
intTestPredict["month_12xtemp_norm"] = intTestPredict["month_12.0"] * intTestPredict["t

# Add workingday x weathersit=1 interaction terms
intTrainPredict["workingdayxweather_1"] = intTrainPredict["workingday"] * intTrainPredi
intTestPredict["workingdayxweather_1"] = intTestPredict["workingday"] * intTestPredict[
```

In [29]:
```
# Fit Interaction OLS model
intModel = sm.OLS(yTrain, intTrainPredict).fit()
intModel.summary()
```

Out[29]:
```
<class 'statsmodels.iolib.summary.Summary'>
"""
                            OLS Regression Results
==============================================================================
Dep. Variable:                  count   R-squared:                       0.670
Model:                            OLS   Adj. R-squared:                  0.623
```

```
Method:                 Least Squares   F-statistic:                     14.31
Date:                Tue, 10 Oct 2017   Prob (F-statistic):           1.07e-48
Time:                        13:29:19   Log-Likelihood:                -2790.7
No. Observations:                 331   AIC:                             5665.
Df Residuals:                     289   BIC:                             5825.
Df Model:                          41
Covariance Type:            nonrobust
==============================================================================
                      coef    std err          t      P>|t|      [0.025      0.975
------------------------------------------------------------------------------
holiday          -504.8692    376.774     -1.340      0.181   -1246.437     236.69
workingday        -78.3221    242.127     -0.323      0.747    -554.878     398.23
temp_norm         793.8768    763.389      1.040      0.299    -708.631    2296.38
atemp_norm        880.3824    715.945      1.230      0.220    -528.745    2289.51
humidity_norm    -675.3295    158.264     -4.267      0.000    -986.826    -363.83
windspeed_norm   -446.4038    149.948     -2.977      0.003    -741.532    -151.27
weather_1.0       923.0406    594.656      1.552      0.122    -247.366    2093.44
weather_2.0      1104.9141    502.004      2.201      0.029     116.866    2092.96
day_of_week_0.0  -462.4486    248.640     -1.860      0.064    -951.824      26.92
day_of_week_1.0  -239.5854    159.457     -1.503      0.134    -553.429      74.25
day_of_week_2.0  -280.3233    188.566     -1.487      0.138    -651.459      90.81
day_of_week_3.0    -3.0325    200.247     -0.015      0.988    -397.160     391.09
day_of_week_4.0  -119.9933    192.772     -0.622      0.534    -499.408     259.42
day_of_week_5.0    59.7432    187.628      0.318      0.750    -309.547     429.03
season_1.0      -1493.1626    505.353     -2.955      0.003   -2487.801    -498.52
season_2.0       -729.5247    549.124     -1.329      0.185   -1810.315     351.26
season_3.0         71.1170    422.825      0.168      0.867    -761.090     903.32
month_2.0        -325.7395    415.794     -0.783      0.434   -1144.107     492.62
month_3.0        -311.7359    465.982     -0.669      0.504   -1228.885     605.41
month_4.0        -429.5823    676.680     -0.635      0.526   -1761.428     902.26
month_5.0       -1024.8594    711.364     -1.441      0.151   -2424.970     375.25
month_6.0       -1466.6541    734.348     -1.997      0.047   -2912.002     -21.30
month_7.0       -1427.6739    798.423     -1.788      0.075   -2999.136     143.78
month_8.0       -1720.6375    791.728     -2.173      0.031   -3278.922    -162.35
month_9.0       -1055.9093    726.079     -1.454      0.147   -2484.983     373.16
month_10.0       -882.2336    692.220     -1.274      0.204   -2244.665     480.19
month_11.0       -773.6133    656.762     -1.178      0.240   -2066.257     519.03
month_12.0       -480.9222   1027.332     -0.468      0.640   -2502.924    1541.08
const            6035.4428    902.323      6.689      0.000    4259.486    7811.40
temp_norm_2     -1796.4144    817.390     -2.198      0.029   -3405.207    -187.62
atemp_norm_2     1167.1361    790.067      1.477      0.141    -387.880    2722.15
humidity_norm_2   -56.3479    155.509     -0.362      0.717    -362.421     249.72
windspeed_norm_2  -37.7429    127.475     -0.296      0.767    -288.641     213.15
temp_norm_3         1.6553    277.479      0.006      0.995    -544.481     547.79
atemp_norm_3     -297.6352    246.540     -1.207      0.228    -782.877     187.60
humidity_norm_3   -14.9630     44.946     -0.333      0.739    -103.425      73.49
windspeed_norm_3   44.3740     65.415      0.678      0.498     -84.376     173.12
temp_norm_4       -44.4857    170.895     -0.260      0.795    -380.843     291.87
```

```
atemp_norm_4            -20.9201     147.604     -0.142      0.887     -311.435      269.59
humidity_norm_4         -23.8429      31.490     -0.757      0.450      -85.822       38.13
windspeed_norm_4        -19.2421      30.292     -0.635      0.526      -78.862       40.37
month_12xtemp_norm       44.3435     714.542      0.062      0.951    -1362.024     1450.71
workingdayxweather_1    165.0265     322.219      0.512      0.609     -469.167      799.22
==============================================================================
Omnibus:                       29.023   Durbin-Watson:                   1.960
Prob(Omnibus):                  0.000   Jarque-Bera (JB):               10.080
Skew:                          -0.099   Prob(JB):                      0.00647
Kurtosis:                       2.168   Cond. No.                     3.92e+16
==============================================================================

Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specif
[2] The smallest eigenvalue is 2.52e-29. This might indicate that there are
strong multicollinearity problems or that the design matrix is singular.
"""
```

In [30]:
```
yHatTest = intModel.predict(intTestPredict)
r2_score(yTest, yHatTest)
```

Out[30]:
```
0.28297793302407059
```

3.4 Answers to Above Questions

- For each continuous predictor X_j, include additional polynomial terms X_j^2, X_j^3, and X_j^4, and fit a multiple regression model to the expanded training set. How does the R^2 of this model on the test set compare with that of the linear model fitted in Part (b) from HW 3? Using a t-test, find out which of estimated coefficients for the polynomial terms are statistically significant at a significance level of 5%.

We found that the R^2 of this model was .277 for the test data set, which clearly outperforms the R^2 score of our HW3 model on the test data set of .249. Using the t-tests provided in the summary above, we found that the only statistically significant coefficient was *temp_norm_2*, which equates to X^2 where X is the normalized continuous variable for temperature.

- Fit a multiple linear regression model with additional interaction terms $\mathbb{I}_{month=12} \times temp$ and $\mathbb{I}_{workingday=1} \times \mathbb{I}_{weathersit=1}$ and report the test R^2 for the fitted model. How does this compare with the R^2 obtained using linear model in Part (b) from HW 3? Are the estimated coefficients for the interaction terms statistically significant at a significance level of 5%?

For this additional model, we found that the R^2 score on the test set was .283, even better than our previous model of .277, and much better than the HW3 model of .249. There are no statistically significant interaction coefficients, as their 95% confidence intervals, as shown above, include 0.

3.5 Part (h): PCA to deal with high dimensionality

We would like to fit a model to include all main effects, polynomial terms up to the 4^{th} order, and all interactions between all possible predictors and polynomial terms (not including the interactions between X_j^1, X_j^2, X_j^3, and X_j^4 as they would just create higher order polynomial terms).

- Create an expanded training set including all the desired terms mentioned above. What are the dimensions of this 'design matrix' of all the predictor variables? What are the issues with attempting to fit a regression model using all of these predictors?
- Instead of using the usual approaches for model selection, let's instead use principal components analysis (PCA) to fit the model. First, create the principal component vectors in python (consider: should you normalize first?). Then fit 5 different regression models: (1) using just the first PCA vector, (2) using the first two PCA vectors, (3) using the first three PCA vectors, etc... Briefly summarize how these models compare in the training set.
- Use the test set to decide which of the 5 models above is best to predict out of sample. How does this model compare to the previous models you've fit? What are the interpretations of this model's coefficients?

```
In [31]: xTest = testPredict
         yTest = testBinaryDf["count"]

         xTrain = trainPredict
         yTrain = trainBinaryDf["count"]

         genPolyTerms = PolynomialFeatures(degree=4, interaction_only=False)

         xTrainPoly = []
         xTestPoly = []

         xTrainPoly.append(genPolyTerms.fit_transform(xTrain))
         xTestPoly.append(genPolyTerms.fit_transform(xTest))

         print("There are {} predictors in this new design matrix.".format(xTrainPoly[0].shape[1
```

```
There are 40920 predictors in this new design matrix.
```

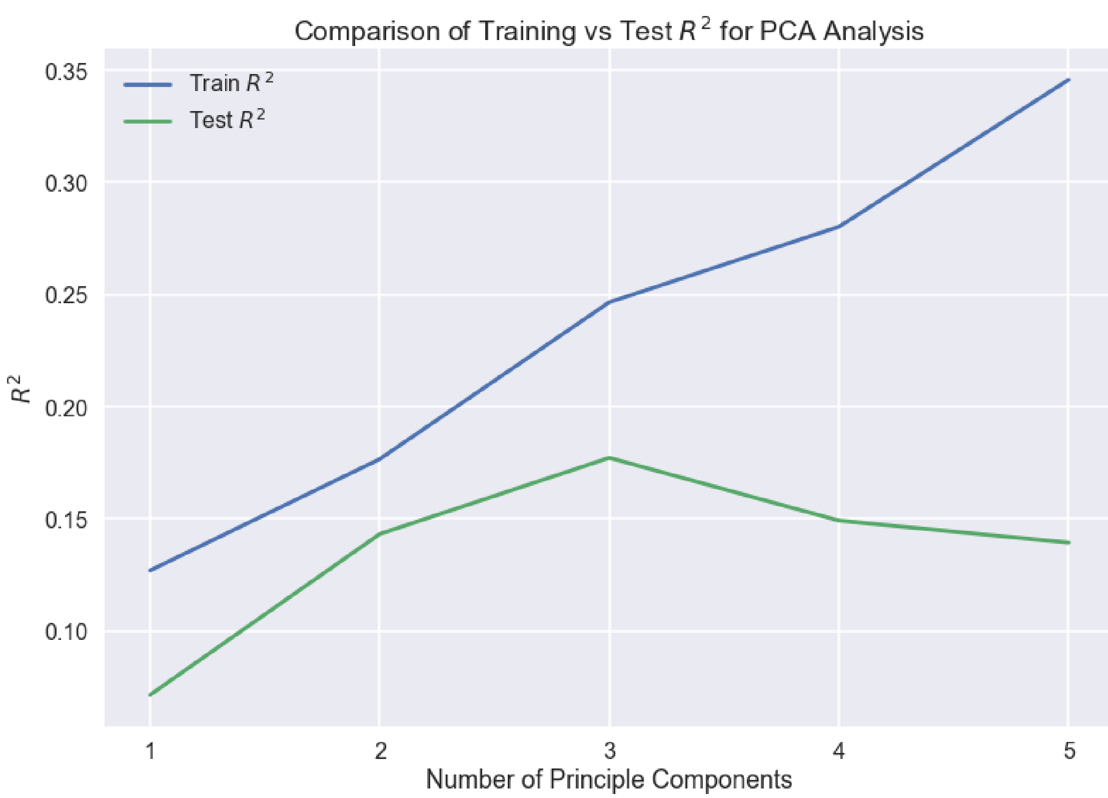
```
In [32]: pcaXTrainVals = []
         pcaXTestVals = []
         for i in range(1,6):
             pca = PCA(n_components=i)
             pca.fit(xTrainPoly[0])
             xPCA = pca.transform(xTrainPoly[0])
             xTestPCA = pca.transform(xTestPoly[0])
             pcaXTrainVals.append(xPCA)
             pcaXTestVals.append(xTestPCA)
```

```
In [33]: trainPCAModels = []
         r2sTrain = []
         r2sTest = []

         for i, data in enumerate(pcaXTrainVals):
             regPCAModel = LinearRegression(fit_intercept=True)
```

```
        regPCAModel.fit(data, yTrain)
        r2sTrain.append(regPCAModel.score(data, yTrain))
        r2sTest.append(regPCAModel.score(pcaXTestVals[i], yTest))
        trainPCAModels.append(regPCAModel)
```

In [34]:
```
fig, ax = plt.subplots()
ax.plot(range(1,6), r2sTrain, label="Train $R^2$")
ax.plot(range(1,6), r2sTest, label="Test $R^2$")
ax.set_xlabel("Number of Principle Components")
ax.set_ylabel("$R^2$")
ax.set_title("Comparison of Training vs Test $R^2$ for PCA Analysis")
plt.xticks(range(1,6), )
ax.legend()

r2sTrain, r2sTest
```

Out[34]:
```
([0.12699183896138022,
  0.17662017642476535,
  0.24654449750664345,
  0.28015860595895636,
  0.34565321930651116],
 [0.07156378309358824,
  0.14324347551193373,
  0.17721903027072172,
  0.14923996544624762,
  0.13943327928477645])
```



```
In [35]: pcaGoalModel = trainPCAModels[2]
         print("The coefficients are: {}.".format(pcaGoalModel.coef_))
         print("The intercept is: {}.".format(pcaGoalModel.intercept_))
```

```
The coefficients are: [-34.95509138 -32.72310621  48.22779015].
The intercept is: 4598.447129909366.
```

3.6 Answers to Above Questions

- Create an expanded training set including all the desired terms mentioned above. What are the dimensions of this 'design matrix' of all the predictor variables? What are the issues with attempting to fit a regression model using all of these predictors?

We can see that there are 40,920 predictor variables in this new design matrix, with 331 rows. One major reason why we would not want to fit a model with this many predictors is because the number of predictors is larger than the number of data points, implying that our model will completely overfit our data. Additionally, we will have collinearity, and model selection (applying stepwise forward algorithms) become intractable.

- Instead of using the usual approaches for model selection, let's instead use principal components analysis (PCA) to fit the model. First, create the principal component vectors in python (consider: should you normalize first?). Then fit 5 different regression models: (1) using just the first PCA vector, (2) using the first two PCA vectors, (3) using the first three PCA vectors, etc... Briefly summarize how these models compare in the training set.

From the above plot, we can see that as the number of principle components included in our model increases, our training R^2 monotonically increases. This makes sense, as we are doing a better job at capturing the variance in our training data with each additional principle component. However, for the test data, we find that we begin to overfit our training data after including the 3 most significant components. This is seen by the concave line plot for the test data above.

- Use the test set to decide which of the 5 models above is best to predict out of sample. How does this model compare to the previous models you've fit? What are the interpretations of this model's coefficients?

From the above, we find that it is best to select the model with 3 principle components. This model is much worse than our previous models, with a R^2 for the test data set of .177. There are no obvious interpretations of this model's coefficients, other than the weightings of each principle component vector. These weightings are [-34.95509138 -32.72310589 48.22779733] respectively. Further, we have a very large positive intercept of 4598.447129909366.

3.7 Part (i): Beyond Squared Error

We have seen in class that the multiple linear regression method optimizes the Mean Squared Error (MSE) on the training set. Consider the following alternate evaluation metric, referred to as the Root Mean Squared Logarthmic Error (RMSLE):

$$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(log(y_i+1)-log(\hat{y}_i+1))^2}.$$

The *lower* the RMSLE the *better* is the performance of a model. The RMSLE penalizes errors on smaller responses more heavily than errors on larger responses. For example, the RMSLE penalizes a prediction of $\hat{y} = 15$ for a true response of $y = 10$ more heavily than a prediction of $\hat{y} = 105$ for a true response of 100, though the difference in predicted and true responses are the same in both cases.

This is a natural evaluation metric for bike share demand prediction, as in this application, it is more important that the prediction model is accurate on days where the demand is low (so that the few customers who arrive are served satisfactorily), compared to days on which the demand is high (when it is less damaging to lose out on some customers).

The following code computes the RMSLE for you:

```
In [36]: #--------  rmsle
         # A function for evaluating Root Mean Squared Logarithmic Error (RMSLE)
         # of the linear regression model on a data set
         # Input:
         #      y_test (n x 1 array of response variable vals in testing data)
         #      y_pred (n x 1 array of response variable vals in testing data)
         # Return:
         #      RMSLE (float)

         def rmsle(y, y_pred):
             # Evaluate sqaured error, against target labels
             # rmsle = \sqrt(1/n \sum_i (log (y[i]+1) - log (y_pred[i]+1))^2)
             rmsle_ = np.sqrt(np.mean(np.square(np.log(y+1) - np.log(y_pred+1))))

             return rmsle_
```

Use the above code to compute the training and test RMSLE for the polynomial regression model you fit in Part (g).

You are required to develop a strategy to fit a regression model by optimizing the RMSLE on the training set. Give a justification for your proposed approach. Does the model fitted using your approach yield lower train RMSLE than the model in Part (g)? How about the test RMSLE of the new model?

Note: We do not require you to implement a new regression solver for RMSLE. Instead, we ask you to think about ways to use existing built-in functions to fit a model that performs well on RMSLE. Your regression model may use the same polynomial terms used in Part (g).

```
In [37]: # your code here
         yTest = testBinaryDf["count"]

         yHatTest = multModel.predict(multTestPredict)
         print("RMSLE for the model in part g: {}".format(rmsle(yTest, yHatTest)))
```

```
RMSLE for the model in part g: 0.5242723327381363
```

```
/Applications/anaconda/lib/python3.6/site-packages/ipykernel_launcher.py:13: RuntimeWarning: inv
  del sys.path[0]
```

```
In [38]: X = multTrainPredict.copy()
         Y = yTrain

         newModel = sm.OLS(list(Y), X).fit()
         yHat = newModel.predict(X)

         error = np.abs(yHat - Y)

         Y = Y.reindex([error.argsort()])
         X = X.reindex([error.argsort()])

         X_aug = X
         Y_aug = Y

         for _ in range(400):
             X_aug = X_aug.append(X[:50])
             Y_aug = Y_aug.append(Y[:50])

         newModel = sm.OLS(list(Y_aug), X_aug).fit()
         yHat = newModel.predict(multTestPredict)
         rmsleVal = rmsle(yTest, yHat)
         print("Our new RMSLE is: {}.".format(rmsleVal))
```

```
Our new RMSLE is: 0.5051747912721489.
```

```
/Applications/anaconda/lib/python3.6/site-packages/ipykernel_launcher.py:13: RuntimeWarning: inv
  del sys.path[0]
```

3.8 Answers to Above Questions

- You are required to develop a strategy to fit a regression model by optimizing the RMSLE on the training set. Give a justification for your proposed approach. Does the model fitted using your approach yield lower train RMSLE than the model in Part (g)? How about the test RMSLE of the new model?

Our strategy to fit a regression model to optimize RMSLE on the training set was the following. We recognized that data points with small absolute errors in an initial fitting of our training data set would decrease the RMSLE. Therefore, we augmented our training data by including data points with small absolute residuals multiple times. This approach intuitively makes sense, as small $|\hat{Y} - Y| \Rightarrow \ln(\hat{Y}+1) - \ln(Y+1)$ will also be small, decreasing our overall RMSLE.

Our new model has an $RMSLE$ value on the test data of .505, which is better than our previous model from part (g)'s score of .524.

3.9 Part (j): Dealing with Erroneous Labels

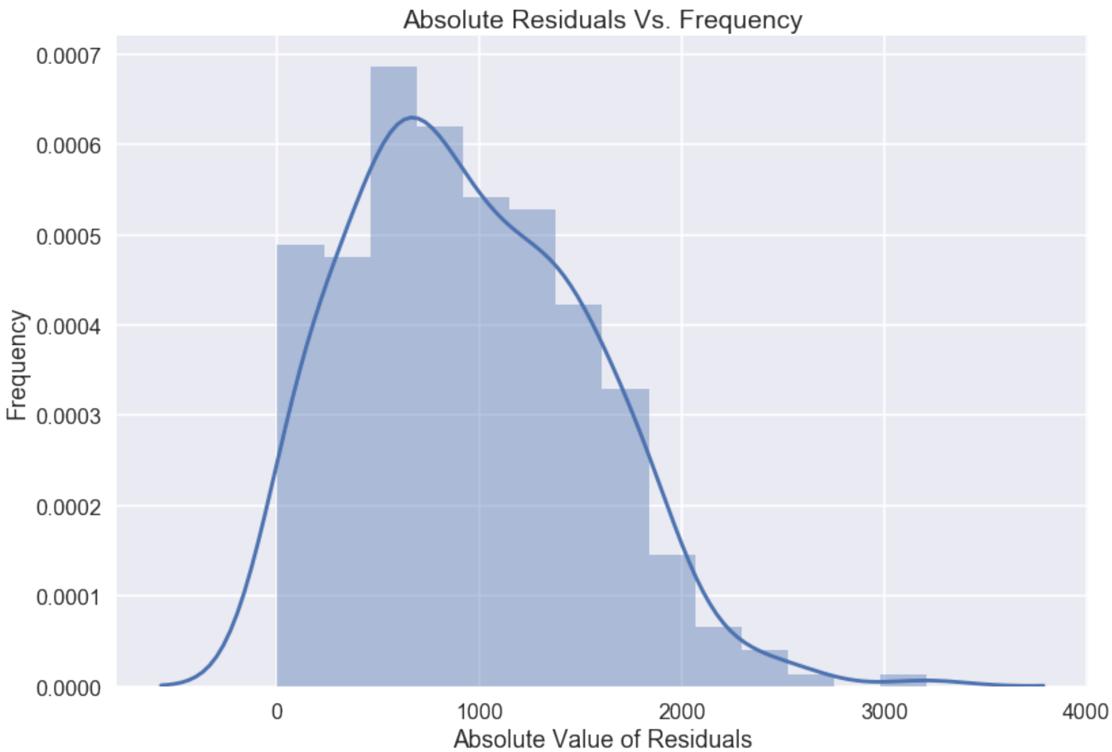
Due to occasional system crashes, some of the bike counts reported in the data set have been recorded manually. These counts are not very unreliable and are prone to errors. It is known that roughly 5% of the labels in the training set are erroneous (i.e. can be arbitrarily different from the true counts), while all the labels in the test set were confirmed to be accurate. Unfortunately, the identities of the erroneous records in the training set are not available. Can this information about presence of 5% errors in the training set labels (without details about the specific identities of the erroneous rows) be used to improve the performance of the model in Part (g)? Note that we are interested in improving the R^2 performance of the model on the test set (not the training R^2 score).

As a final task, we require you to come up with a strategy to fit a regression model, taking into account the errors in the training set labels. Explain the intuition behind your approach (we do not expect a detailed mathematical justification). Use your approach to fit a regression model on the training set, and compare its test R^2 with the model in Part (g).

Note: Again, we do not require you to implement a new regression solver for handling erroneous labels. It is sufficient that you to come up with an approach that uses existing built-in functions. Your regression model may use the same polynomial terms used in Part (g).

In [39]:
```
# identify absolute error

multModel = sm.OLS(yTrain, multTrainPredict).fit()
yHatTrain = multModel.predict(multTrainPredict)

errors =  yTrain - yHatTrain
abserrors = np.array(abs(errors))

fig, ax = plt.subplots(1)
ax.set_title("Absolute Residuals Vs. Frequency")
ax.set_ylabel("Frequency")
ax.set_xlabel("Absolute Value of Residuals")
sns.distplot(abserrors)
```

Out[39]: <matplotlib.axes._subplots.AxesSubplot at 0x111dc1978>



In [40]:
```
dropIndices = abserrors.argsort()[-int(len(abserrors)*0.05):][::-1]

adjYTrain = yTrain.drop(yTrain.index[dropIndices])
adjXTrain = multTrainPredict.drop(multTrainPredict.index[dropIndices])
adjMultModel = sm.OLS(adjYTrain, adjXTrain).fit()
adjMultModel.summary()
```

Out[40]:
```
<class 'statsmodels.iolib.summary.Summary'>
"""
                            OLS Regression Results
==============================================================================
Dep. Variable:                  count   R-squared:                       0.718
Model:                            OLS   Adj. R-squared:                  0.678
Method:                 Least Squares   F-statistic:                     17.93
Date:                Tue, 10 Oct 2017   Prob (F-statistic):           3.05e-55
Time:                        13:29:30   Log-Likelihood:                -2625.6
No. Observations:                 315   AIC:                             5331.
Df Residuals:                     275   BIC:                             5481.
Df Model:                          39
Covariance Type:            nonrobust
==================================================================================
                     coef    std err          t      P>|t|      [0.025      0.975]
----------------------------------------------------------------------------------
```

holiday	-89.0664	363.130	-0.245	0.806	-803.935	625.802
workingday	85.7392	152.585	0.562	0.575	-214.643	386.122
temp_norm	753.7641	698.454	1.079	0.281	-621.233	2128.761
atemp_norm	931.9529	655.442	1.422	0.156	-358.368	2222.274
humidity_norm	-695.2858	144.789	-4.802	0.000	-980.322	-410.250
windspeed_norm	-443.0108	138.341	-3.202	0.002	-715.353	-170.669
weather_1.0	1007.8855	509.110	1.980	0.049	5.638	2010.133
weather_2.0	1082.5915	463.259	2.337	0.020	170.607	1994.576
day_of_week_0.0	-340.7946	232.970	-1.463	0.145	-799.425	117.836
day_of_week_1.0	-202.8532	149.029	-1.361	0.175	-496.235	90.529
day_of_week_2.0	-207.6025	172.805	-1.201	0.231	-547.791	132.586
day_of_week_3.0	138.3122	184.038	0.752	0.453	-223.990	500.615
day_of_week_4.0	112.0110	185.816	0.603	0.547	-253.791	477.813
day_of_week_5.0	156.8052	172.188	0.911	0.363	-182.168	495.779
season_1.0	-1662.8420	429.543	-3.871	0.000	-2508.452	-817.232
season_2.0	-675.8582	493.064	-1.371	0.172	-1646.518	294.802
season_3.0	226.2033	385.309	0.587	0.558	-532.326	984.733
month_2.0	-248.0666	388.167	-0.639	0.523	-1012.224	516.091
month_3.0	-440.3675	425.067	-1.036	0.301	-1277.166	396.430
month_4.0	-492.6351	603.950	-0.816	0.415	-1681.588	696.318
month_5.0	-1301.7164	635.376	-2.049	0.041	-2552.536	-50.897
month_6.0	-1853.3696	656.642	-2.822	0.005	-3146.053	-560.686
month_7.0	-1693.9734	701.678	-2.414	0.016	-3075.316	-312.631
month_8.0	-2041.3922	699.262	-2.919	0.004	-3417.979	-664.805
month_9.0	-1316.2651	617.398	-2.132	0.034	-2531.692	-100.838
month_10.0	-1272.8666	574.251	-2.217	0.027	-2403.353	-142.380
month_11.0	-960.2166	550.751	-1.743	0.082	-2044.441	124.008
month_12.0	-618.9551	447.518	-1.383	0.168	-1499.952	262.042
const	6165.5547	779.588	7.909	0.000	4630.837	7700.273
temp_norm_2	-2178.4066	754.456	-2.887	0.004	-3663.650	-693.163
atemp_norm_2	1441.5058	728.145	1.980	0.049	8.060	2874.952
humidity_norm_2	-72.8165	143.386	-0.508	0.612	-355.090	209.457
windspeed_norm_2	-70.4969	116.980	-0.603	0.547	-300.787	159.793
temp_norm_3	28.2302	252.891	0.112	0.911	-469.618	526.078
atemp_norm_3	-327.9724	225.474	-1.455	0.147	-771.847	115.903
humidity_norm_3	-22.5567	41.820	-0.539	0.590	-104.886	59.772
windspeed_norm_3	54.3955	60.873	0.894	0.372	-65.442	174.233
temp_norm_4	-2.6787	157.059	-0.017	0.986	-311.868	306.511
atemp_norm_4	-51.0898	135.467	-0.377	0.706	-317.775	215.595
humidity_norm_4	-23.4383	28.842	-0.813	0.417	-80.217	33.341
windspeed_norm_4	-18.2169	27.861	-0.654	0.514	-73.065	36.631

==

Omnibus:	53.297	Durbin-Watson:	1.956
Prob(Omnibus):	0.000	Jarque-Bera (JB):	12.734
Skew:	-0.055	Prob(JB):	0.00172
Kurtosis:	2.021	Cond. No.	3.14e+16

==

```
Warnings:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specif
[2] The smallest eigenvalue is 3.81e-29. This might indicate that there are
strong multicollinearity problems or that the design matrix is singular.
"""
```

In [41]:
```
yHatAdjTest = adjMultModel.predict(multTestPredict)
r2_score(yTest, yHatAdjTest)
```

Out[41]:
```
0.26553825406157139
```

3.10 Answer to Above Questions

- As a final task, we require you to come up with a strategy to fit a regression model, taking into account the errors in the training set labels. Explain the intuition behind your approach (we do not expect a detailed mathematical justification). Use your approach to fit a regression model on the training set, and compare its test R^2 with the model in Part (g).

Our strategy for the above problem was the following. We wanted to find the values in our training data set where the absolute value of their residuals were particularly large. By excluding the top 5% largest absolute residuals, we ensure that any erroneous entries are not outliers skewing our model unfavorably. We recognize that there is a chance we have not removed exactly all of the errors, but in the event that the errors are clustered with the majority of our correct data, our model should still accurately predict our training data set.
This hypothesis is supported by the fact that our R^2 on the test data set did not significantly decrease from our previous model with the outliers in the training data set. Our new R^2 is .266, which is slightly lower than .277 from our model in part *g*.

In [ ]:

In [ ]:

In [ ]:

In [ ]:

In [ ]: