Bayesian Inference in Larger Models

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1 Inference in Larger Graphical Models: Student Performance Estimation

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2 Introduction

In this notebook, I look at predicting students outcomes using Bayesian linear regression. Student grades are influenced by many factors, and using a linear model allows us to determine the relationships between these variables and the final performance.

3 Problem Statement

This is a supervised regression problem: we have labels, the final performance of students, that we wish to predict from a set of known features. The labels are continuous (from 1-20) which makes this a regression problem (we could also formulate it as a classification with 20 discrete classes but we will treat the grades as continuous). There are many standard machine learning approaches that can be used to create a model mapping the features in the training data to the labels. These models can be easily built in scikit-learn and then tested against a hold-out testing set. We will look at several standard machine learning models in addition to Bayesian Linear Regression for comparison.

3.1 Dataset

The data about student performance was collected from a Portuguese secondary school and is available at the UCI machine learning repository. The target variable to predict is G3, the final student grade ranging from 0 to 20. There are 30 features in the original data, but in order to reduce dimensionality, I calculate the Pearson Correlation Coefficient between all the features and the response and only retain the features with a correlation coefficient greater than 0.2 in absolute magnitude. Given that we are performing linear regression, selecting variables that are highly correlated with the response should improve the performance of the model. Before perfomring the correlation analysis, I one-hot encode all the variables.

3.1.1 Features

The final set of five features selected are as follows:

- 1. failures: number of previous class failures, numeric, the number of classes is 1 <= n < 3 else 4.
- 2. higher_yes: binary 0 if the student does not want to pursue higher education and 1 if the student does want to pursue higher education.
- 3. Medu: Mother's education, numeric, 0 = none, 1 = primary education (4th grade), 2 = 5th to 9th grade, 3 = secondary education, 4 = higher education
- 4. studytime: time of studying per week, numeric, 1: <2 hours, 2: 2 to 5 hours, 3: 5 to 10 hours, 4: >10 hours.
- 5. Dalc: daily alcohol consumption during the week, numeric, 1 very low to 5 very high

3.2 Bayesian Network

In effect, our final network looks like this:

We have five different variables, all of which affect the final grade to some extent. Instead of specifying prior probabilities for each feature and conditional probabilities between the response (final score) and the feature, we will use Bayesian Linear Regression to determine the weights between the features and the response. This is taking a machine learning approach to the problem, but we will use Bayesian Inference to create our model.

4 Bayesian Linear Regression

The standard linear regression is

$$Y = X\beta + \epsilon$$

Where Y is the target, X is the predictor matrix, β is the weights vector, and ϵ is an error term (assumed to be normally distributed. The weights are found using ordinary least squares to minimum the residual sum of squares between the observations (training data) and the fit.

In a Bayesian framework, Linear Regression takes the form

$$Y \sim \mathcal{N}(X\beta, \sigma^2)$$

Where Y is a random variable with each data point distributed according to a normal distribution. The mean of the normal distribution comes from the data points multiplied by the weights vector β with a variance of σ^2 .

The Bayesian Linear Regression framework has two main advantages:

- Priors: Any previous knowledge about the problem can be quantified by placing prior probabilities on the model parameters. For example, if we believe one of the explanatory variables has a one-to-one linear relationship with the response, then we can assign the intial starting value of 1 to the corresponding weight.
- Uncertainty: Bayesian inference using Markov Chain Monte Carlo does not yield a single estimate for each weight, but rather a posterior *distribution* from which we can draw conclusions about how likely different values of the weights β are in our model. With fewer data points, there will be more uncertainty in β and the posteriors distributions will thus be very wide.

4.1 Comparison to other Models

import pandas as pd import numpy as np np.random.seed(42)

%matplotlib inline

In [1]: # Pandas and numpy for data manipulation

import matplotlib.pyplot as plt

Matplotlib and seaborn for plotting

We will start off by solving this regression problem using several standard machine learning models from scikit-learn. This library makes creating, training, and evaluating models very simple.

```
import seaborn as sns
        from IPython.core.pylabtools import figsize
In [2]: # Standard ML Models for comparison
        from sklearn.linear_model import LinearRegression
        from sklearn.linear_model import ElasticNet
        from sklearn.ensemble import RandomForestRegressor
        from sklearn.ensemble import ExtraTreesRegressor
        from sklearn.ensemble import GradientBoostingRegressor
        from sklearn.svm import SVR
        # Splitting data into training/testing
        from sklearn.model_selection import train_test_split
        from sklearn.preprocessing import MinMaxScaler
        # Metrics
        from sklearn.metrics import mean_squared_error
In [3]: # PyMC3 for Bayesian Inference
        import pymc3 as pm
        # Set number of draws for sampling
        NDRAWS = 2000
WARNING (theano.tensor.blas): Using NumPy C-API based implementation for BLAS functions.
```

4.2 Read in Data and Examine

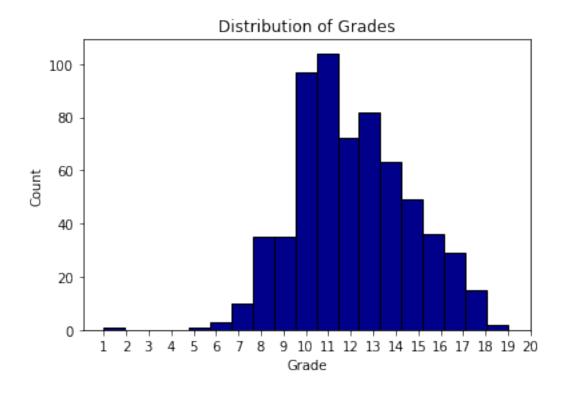
recorded in a math class.

We are using data collected from a Portuguese secondary (high) school. The scores used here were

```
# Filter out grades that were 0
        math = math[math['G3'] != 0]
        math.head()
                        age address famsize Pstatus
Out[4]:
           school sex
                                                        Medu
                                                              Fedu
                                                                          Mjob
                                                                                     Fjob ... \
        0
               GP
                         18
                                   U
                                          GT3
                                                            4
                                                                      at home
                                                                                  teacher ...
                     F
                                                      Α
        1
               GP
                     F
                         17
                                   U
                                          GT3
                                                     Τ
                                                            1
                                                                   1
                                                                      at_home
                                                                                    other ...
        2
                                                      Т
               GP
                     F
                                   U
                                          LE3
                                                                      at home
                                                                                    other ...
                         15
                                                            1
                                                                   1
         3
               GP
                     F
                         15
                                   U
                                          GT3
                                                      Т
                                                            4
                                                                   2
                                                                       health
                                                                                services ...
         4
               GP
                     F
                                   U
                                          GT3
                                                      Т
                                                            3
                                                                   3
                                                                         other
                         16
                                                                                    other ...
           famrel freetime
                              goout
                                     Dalc
                                            Walc health absences
                                                                     G1
                                                                          G2
                                                                              G3
        0
                4
                          3
                                  4
                                                1
                                                        3
                                                                      0
                                         1
                                                                          11
                                                                              11
         1
                5
                           3
                                  3
                                         1
                                                1
                                                        3
                                                                  2
                                                                      9
                                                                          11
                                                                              11
        2
                4
                           3
                                  2
                                         2
                                                        3
                                                3
                                                                  6
                                                                     12
                                                                              12
                                                                         13
         3
                3
                           2
                                  2
                                                        5
                                         1
                                                1
                                                                  0
                                                                     14
                                                                          14
                                                                              14
         4
                4
                           3
                                  2
                                                2
                                                        5
                                         1
                                                                     11
                                                                          13
                                                                              13
         [5 rows x 33 columns]
```

We can look at the distribution of the parameter of interest, the final grade using a summary and a histogram.

```
In [5]: math['G3'].describe()
Out[5]: count
                 634.000000
        mean
                  12.187697
        std
                   2.691824
        min
                   1.000000
        25%
                  10.000000
        50%
                  12.000000
        75%
                  14.000000
                  19.000000
        max
        Name: G3, dtype: float64
In [6]: # Histogram of final grades
        plt.hist(math['G3'], edgecolor = 'k', color = 'darkblue', bins = 19)
        plt.xlabel('Grade'); plt.ylabel('Count'); plt.title('Distribution of Grades');
        plt.xticks(range(1, 21));
```



5 Data Preparation

Data preparation will consist of a few steps:

- 1. One-hot encoding of categorical variables
- 2. Finding the most correlated variables with the response (final grade)
- 3. Split the data into training and testing sets for model fitting and evaluation

```
In [7]: def format_data(df):
    # Targets are final grade of student
    labels = df['G3']
    # Drop the school and the grades from features
    df = df.drop(columns=['school', 'G1', 'G2', 'G3'])

# One-Hot Encoding of Categorical Variables
    df = pd.get_dummies(df)

df['y'] = list(labels)

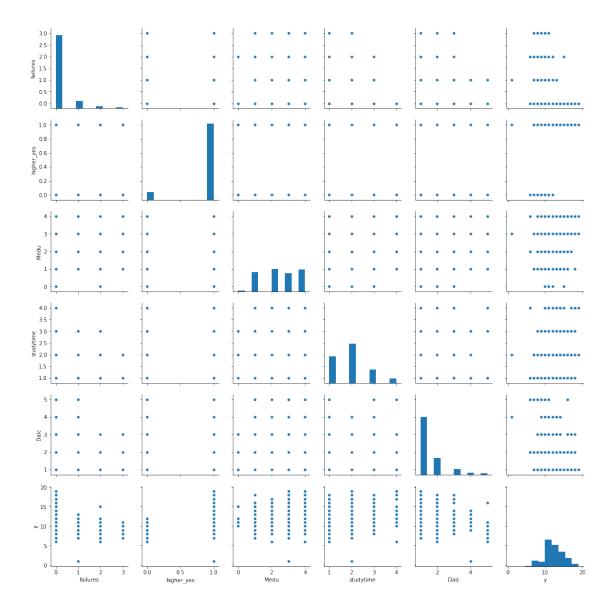
most_correlated = df.corr().abs()['y'].sort_values(ascending=False)

# Keep correlations greater than 0.2 in absolute value
most_correlated = most_correlated[most_correlated >= 0.2][1:]
```

```
df = df.ix[:, most_correlated.index]
            df = df.drop(columns = 'higher_no')
            # Split into training/testing sets with 25% split
            X_train, X_test, y_train, y_test = train_test_split(df, labels,
                                                                  test size = 0.25,
                                                                random state=42)
            return X_train, X_test, y_train, y_test
In [8]: X_train_math, X_test_math, y_train_math, y_test_math = format_data(math)
        X_train_math.head()
Out[8]:
             failures higher_yes Medu studytime
        619
                    0
                                       3
                                                  2
                                 1
                                                        1
        596
                                                  2
                    0
                                 1
                                       4
                                                        1
        550
                    0
                                 1
                                       2
                                                  2
                                                        2
        516
                    0
                                 1
                                       4
                                                  2
                                                        2
        472
                    0
                                       2
                                                  1
                                                        1
                                 1
```

There are 6 variables in the final dataset, although two are one-hot encoding of the same variable. From these six variables, we will try to create a linear regression model that is able to predict student performance.

5.1 Pairplot of Final Variables



6 Evaluate Standard Machine Learning Models for a Benchmark

We can try several standard machine learning models to compare against the final model from Bayesian Linear Regression. We will use the following models:

- 1. Standard Linear Regression
- 2. Elastic Net Linear Regression with an L1 ratio of 0.5
- 3. A Random Forest Regression with 50 trees
- 4. An Extra Trees Regression with 50 trees
- 5. Support Vector Machine Regressor with rbf kernel, a degree of 3, a C penalty of 1, and auto for gamma
- 6. Gradient Boosting Regressor with 20 trees

The overall baseline will simply be guessing the median grade of the training final scores as the final score for all training examples

6.1 Metrics

We will use two metrics to evaluate models:

- Root Mean Squared Error (RMSE): the square root of the average squared error, has the same units as the target variable (grade)
- Median Absolute Percentage Error (MAPE): the fractional error of the estimate, multiply the MAPE by 100 and subtract from 100 to get an estimate of accuraccy.

These metrics will be used to compare the various models for performance. This is no one single best metric for regression and that is why we use two different measures.

```
In [10]: def evaluate(X_train, X_test, y_train, y_test):
             # Names of models
             model_name_list = ['Linear Regression', 'ElasticNet Regression',
                               'Random Forest', 'Extra Trees', 'SVM',
                                'Gradient Boosted', 'Baseline']
             # Instantiate the models
             model1 = LinearRegression()
             model2 = ElasticNet(alpha=1.0, l1_ratio=0.5)
             model3 = RandomForestRegressor(n_estimators=50)
             model4 = ExtraTreesRegressor(n_estimators=50)
             model5 = SVR(kernel='rbf', degree=3, C=1.0, gamma='auto')
             model6 = GradientBoostingRegressor(n_estimators=20)
             # Dataframe for results
             results = pd.DataFrame(columns=['rmse', 'mape'], index = model_name_list)
             # Train and predict with each model
             for i, model in enumerate([model1, model2, model3, model4, model5, model6]):
                 model.fit(X_train, y_train)
                 predictions = model.predict(X_test)
                 # Metrics
                 mse = mean_squared_error(y_test, predictions)
                 rmse = np.sqrt(mse)
                 mape = np.median(np.divide(abs(predictions - y_test), y_test, where= y_test!=
                 # Insert results into the dataframe
                 model_name = model_name_list[i]
                 results.ix[model_name, :] = [rmse, mape]
             # Median Value Baseline Metrics
             baseline_mse = np.mean((np.median(y_train_math) - y_test) ** 2)
```

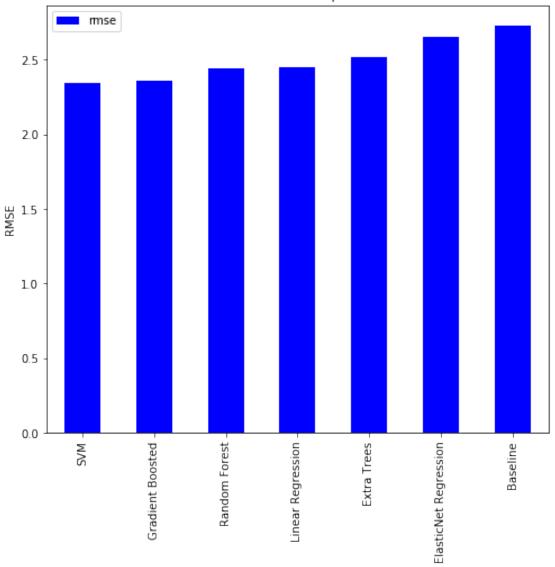
baseline_rmse = np.sqrt(baseline_mse)

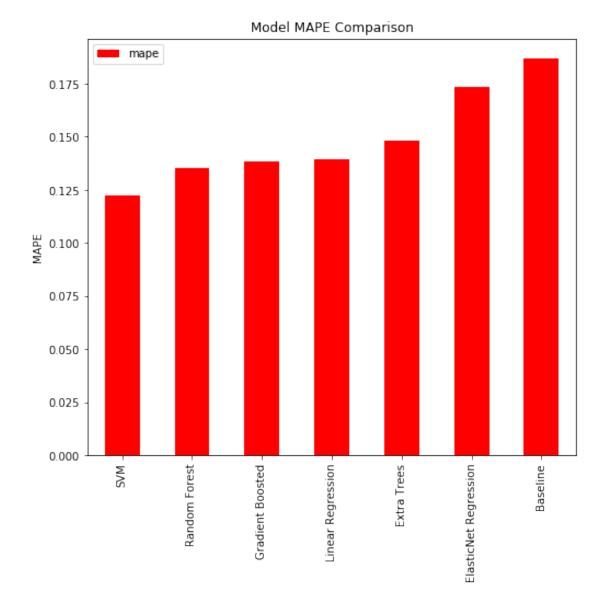
```
baseline_mape = np.median(np.divide(abs(np.mean(y_train) - y_test), y_test, where
results.ix['Baseline', :] = [baseline_rmse, baseline_mape]
return results

In [11]: math_results = evaluate(X_train_math, X_test_math, y_train_math, y_test_math)
```

6.2 Machine Learning Model Results







From the metrics, we can see that the Support Vector Machine Regression performs the best followed by the tree base learning methods. All methods perform better than the median baseline. I did not do any hyperparameter tuning with these models, and we are only using them as a baseline for comparison.

7 Implementing Bayesian Linear Regression

We will be using the GLM.from_formula function in PyMC3 which means we need to create a formula relating the explanatory variables (the features) to the response (the final grade). The GLM.from_formula function call uses the R formula syntax which is shown below. When the model performs inference, it will draw samples from the posterior for each of the variables in the formula, along with an intercept and a variance.

7.0.1 Formula for Linear Regression

```
In [14]: formula
Out[14]: 'y ~ failures + higher_yes + Medu + studytime + Dalc'
```

Now, we can create the model using PyMC3 and perform Markov Chain Monte Carlo to sample from the posterior. The function GLM.from_formula parses the formula string, adds a random variable for each regressor and a likelihood for each random variable which by default is a normal distribution. The function then initializes the parameters (weights, β) to sensible starting points using a frequentists estimate provided by statsmodels.

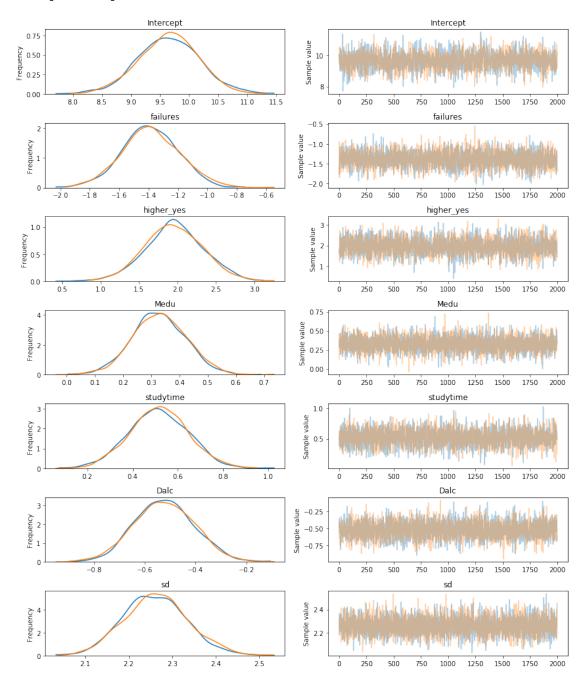
After we perform the sampling, we can examine the varibles from the trace to make predictions and examine the weights of different variables. This model is called the normal model because it assumes the features are drawn from normal distributions, an assumption we will alter in a later iteration.

This model uses relies on PyMC3 for auto-assignment of the sampler. In this case, the model uses the No-UTurn Sampling method (NUTS) which is a special case of Hamiltonian Monte Carlo (HMC)) sampling. Hamiltonian Monte Carlo methods avoid the common random walk behavior of Markov Chain Monte Carlo algorithms by taking steps informed by the first-order gradient. NUTS automatically stops when it begins to double back and retrace steps (No-UTurn) and is generally more efficient than Hamiltonian Monte Carlo which is in turn more efficient than Markov Chain Monte Carlo. HMC converges more quickly than standard MCMC because it avoids the random walk behavior and is an informed sampling method.

8 Examine Results

Rather than provide us with a single estimate for each of the weights, Markov Chain Monte Carlo sampling gives us a distribution of samples for every model parameter. There are many tools available in PyMC3 for examining the results of a model run. For a start, we can use pm.traceplot to examine the distribution of every variable sampled by the model.

In [16]: pm.traceplot(normal_trace);

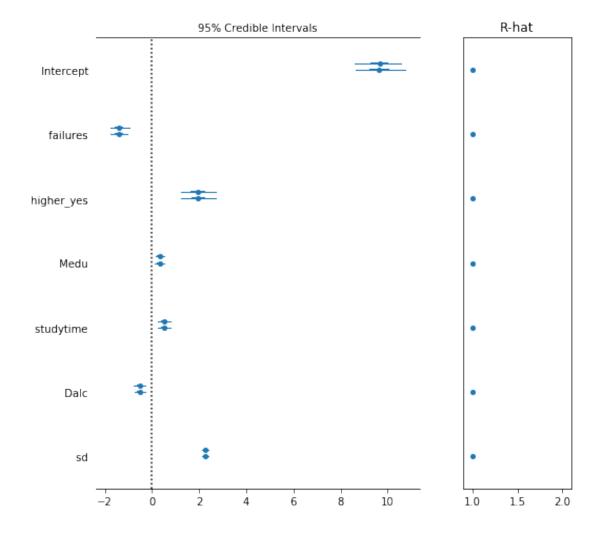


The left side of the traceplot is the marginal posterior: the values for the variable are on the x-axis with the probability for the variable (as determined by sampling) on the y-axis. The different colored lines indicate that we performed two chains of Markov Chain Monte Carlo. From the left side we can see that there is a range of values for each weight. The right side shows the different sample values drawn as the sampling process runs.

Another method built into PyMC3 for examinig trace results is the forestplot which shows the distribution of each sampled parameter. This allows us to see the uncertainty in each sample. The

forestplot is easily constructed from the trace using pm.forestplot.

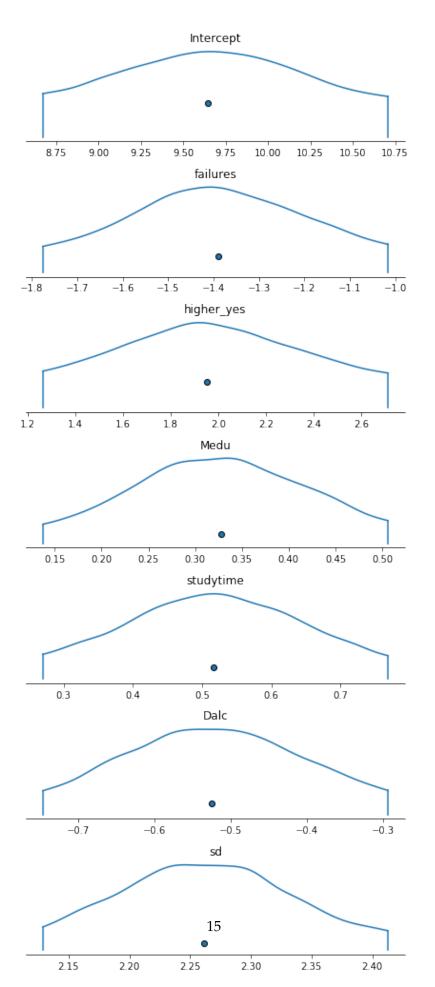
In [17]: pm.forestplot(normal_trace);



From the forest plot we can see the most likely value of the parameter (the dot) as well as the 95% confidence interval for the parameter. The intercept and higher_yes have larger uncertainty compared to the other variables. When we go to make predictions, we can estimate a single number using the most likely value and a range of possible values using all of the samples.

A third method PyMC3 offers for examining the trace of a sampling run is the density plot. This shows the kernel density estimate for each parameter (or the histogram for discrete variables). This again allows us to visualize the distribution of samples.

In [18]: pm.densityplot(normal_trace);



9 Interpretations of Weights

Based on the sign and location of the weights, we can make the following inferences regarding the features in our dataset:

- Previous class failures are negatively related to the students final grade
- Higher education ambitions are positively related to the students grade
- The mother's education level is positively related to the students final grade
- Studying time per week is positively related to the students final grade
- Alcohol consumption during the week is negatively related to the students final grade

9.1 Make Predictions Using Most Likely Values

Variable: sd Median weight in model: 2.2607

Now, we can make predictions for students outcomes using the trace samples. To come up with a single estimate, we take the mean of all the parameter samples.

```
In [20]: def evaluate_trace(trace, X_train, X_test, y_train, y_test, model_results):
    # Dictionary of all sampled values for each parameter
    var_dict = {}
    for variable in trace.varnames:
        var_dict[variable] = trace[variable]

# Results into a dataframe
    var_weights = pd.DataFrame(var_dict)

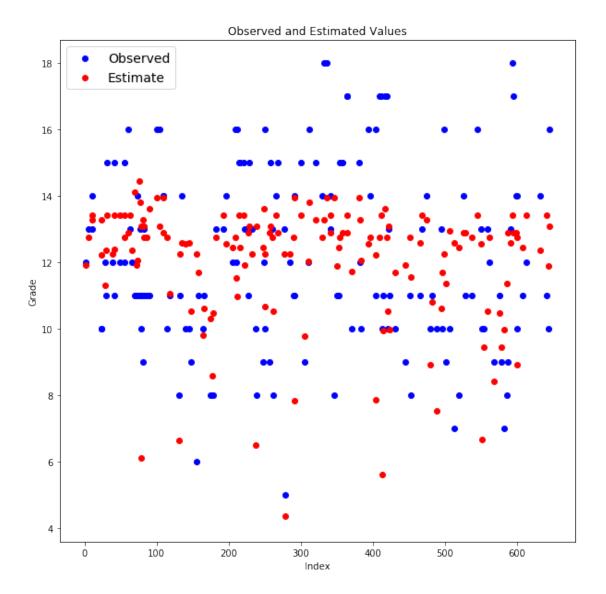
# Means for all the weights
    var_means = var_weights.mean(axis=0)

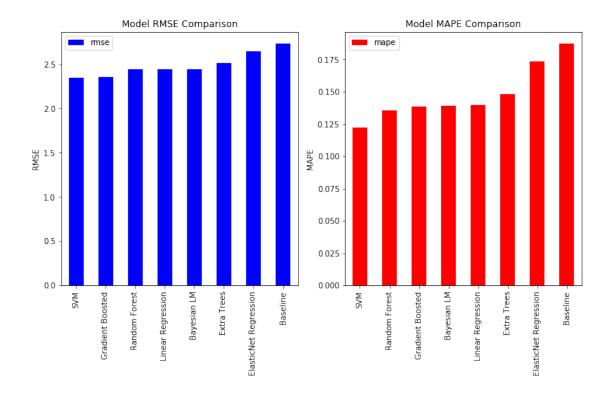
# Create an intercept column
    X_test['Intercept'] = 1
```

```
X_test = X_test.ix[:, names]
             var_means = var_means[names]
             # Calculate estimate for each test observation using the average weights
             results = pd.DataFrame(index = X_test.index, columns = ['estimate'])
             for row in X_test.iterrows():
                 results.ix[row[0], 'estimate'] = np.dot(np.array(var_means), np.array(row[1])
             # Metrics
             actual = np.array(y_test)
             errors = results['estimate'] - actual
             rmse = np.sqrt(mean_squared_error(results['estimate'], actual))
             mape = np.median(abs(errors) / actual)
             print('Model RMSE: {:.4f}\nModel MAPE: {:.4f}'.format(rmse, mape))
             # Plot the observations and predictions
             figsize(10, 10)
             plt.scatter(results.index, actual, label = 'Observed', color = 'blue')
             plt.scatter(results.index, results['estimate'], label = 'Estimate', color = 'red'
             plt.legend(prop={'size': 14}); plt.xlabel('Index'); plt.ylabel('Grade');
             plt.title('Observed and Estimated Values')
             plt.show()
             # Add the results to the comparison dataframe
             model_results.ix['Bayesian LM', :] = [rmse, mape]
             # Plot root mean squared error of all models
             plt.figure(figsize=(12, 6))
             ax = plt.subplot(1, 2, 1)
             model_results.sort_values('rmse', ascending = True).plot.bar(y = 'rmse', color =
             plt.title('Model RMSE Comparison'); plt.ylabel('RMSE')
             # Plot median absolute percentage error of all models
             ax = plt.subplot(1, 2, 2)
             model_results.sort_values('mape', ascending = True).plot.bar(y = 'mape', color =
             plt.title('Model MAPE Comparison'); plt.ylabel('MAPE');
             plt.show();
             return results
In [21]: results = evaluate_trace(normal_trace, X_train_math, X_test_math, y_train_math, y_tes
Model RMSE: 2.4474
```

Align names of the test observations and means

names = X_test.columns





Our first attempt at creating a Bayesian Generalized Linear Model does not do that well in comparison to other models. To improve the model, we could draw more samples or try selecting additional features.

10 Query Model

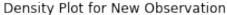
We can now make predictions from the model by passing in a new observation. As the trace contains every sample drawn from the posterior for every weight, we can calculate an entire range of estimates instead of a single number. This shows that there is uncertainty in our estimate.

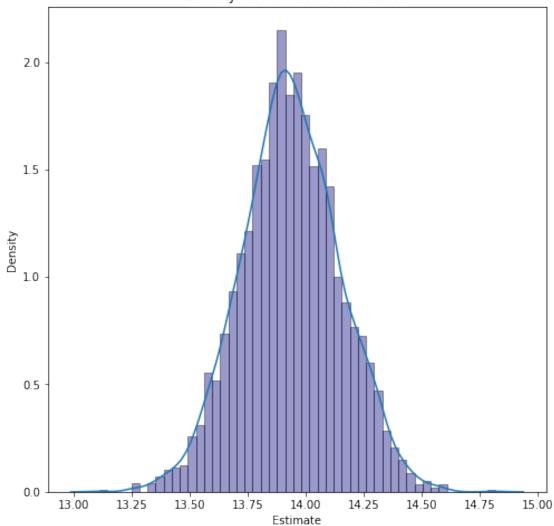
```
In [22]: def query_model(trace, new_observation):
    # Dictionary of all sampled values for each parameter
    var_dict = {}
    for variable in trace.varnames:
        var_dict[variable] = trace[variable]

# Results into a dataframe
    var_weights = pd.DataFrame(var_dict)

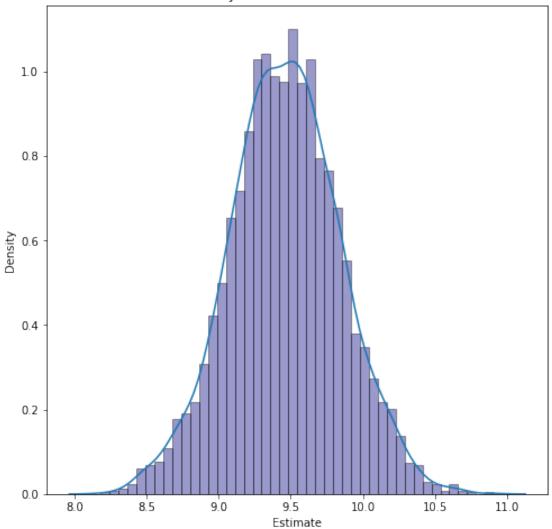
weights = np.array(var_weights.ix[:, observation.columns])
    estimates = np.dot(weights, np.array(new_observation).reshape(6, 1))

plt.figure(figsize(8, 8))
```







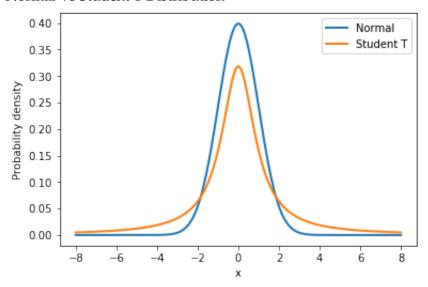


The model estimations seem reasonable and are in line with our intuitions about what influences grades. Moreover, the model predictions take on a range of values which reflects the uncertainty in any real-world prediction. The benefit of Bayesian Inference is that we can show that uncertainty by displaying a range of possible answers instead of a single value.

11 Student T Prior Distribution

In order to make our model more robust to outliers, we can use a different distribution, other than the default of normal, for the prior for the parameters. We can try the Student T Distribution, which has more weight in the tails, meaning the values further from the mean have a higher probability than in a Normal Distribution. This distribution should limit the effect of outliers on the model.

Normal Vs Student T Distribution

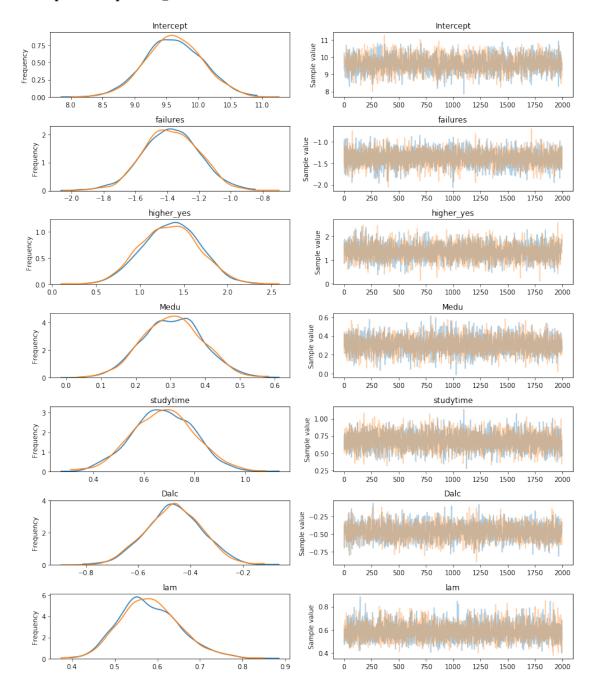


To change the prior distribution in our PyMC3 model, we only have to make a family and pass in to the pm.GLM.from_formula function call. The function then knows to sample from the T distribution rather than from the normal for all the samples.

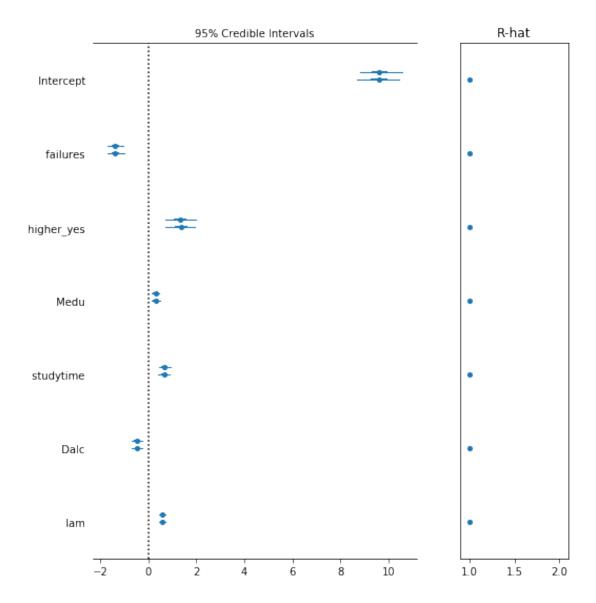
```
In [25]: formula
Out [25]: 'y ~ failures + higher_yes + Medu + studytime + Dalc'
In [26]: X_train_math['y'] = list(y_train_math)
         with pm.Model() as t_model:
             family = pm.glm.families.StudentT()
             pm.GLM.from_formula(formula,
                                 data = X_train_math, family = family)
             # Sample from the posterior
             t_trace = pm.sample(draws=NDRAWS, tune=500, njobs = -1)
Auto-assigning NUTS sampler...
Initializing NUTS using jitter+adapt_diag...
Sequential sampling (2 chains in 1 job)
NUTS: [lam_log__, Dalc, studytime, Medu, higher_yes, failures, Intercept]
100%|| 2500/2500 [00:21<00:00, 117.44it/s]
100%|| 2500/2500 [00:17<00:00, 142.89it/s]
The acceptance probability does not match the target. It is 0.8834000488954877, but should be
```

11.1 Investigate Trace

In [27]: pm.traceplot(t_trace);



In [28]: pm.forestplot(t_trace);

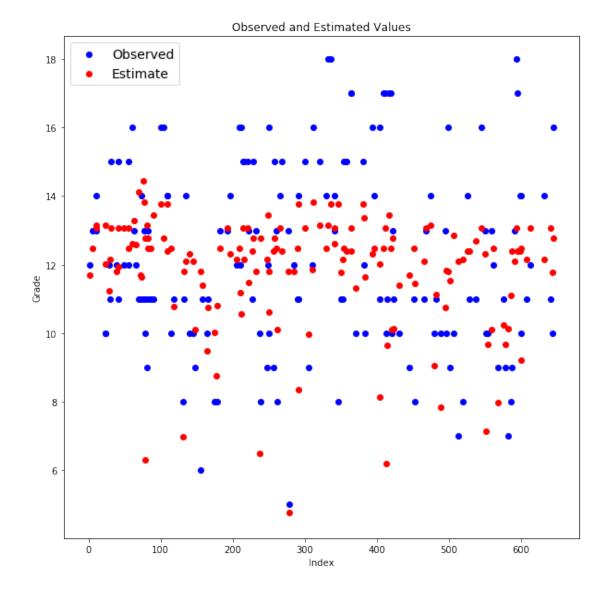


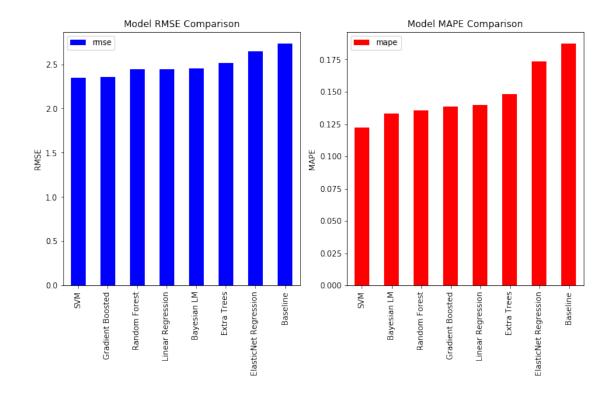
The distributions again show the spread of each parameter sampled during the model run. The intercept and higher_yes variables have the highest amount of uncertainty as was observed for the model using a normal prior distribution.

11.2 Evaluate the New Model

```
In [29]: results = evaluate_trace(t_trace, X_train_math, X_test_math, y_train_math, y_test_math
```

Model RMSE: 2.4486 Model MAPE: 0.1330

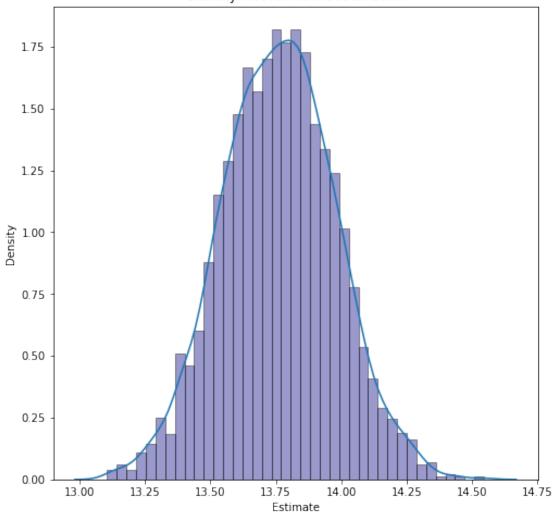


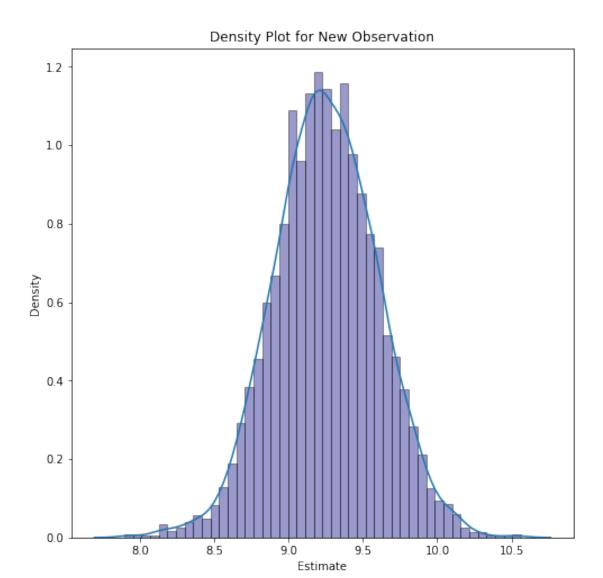


The t-distribution metrics are nearly identical to those from the normal distribution. As the number of samples/datapoints increases, the prior has less and less impact on the final results because the likelihoods come to dominate the parameters drawn from the posterior. We can do the same querying of the new model to view the predictions for a new student.

11.3 Query T-Distribution Model

Density Plot for New Observation





There is some variation between the t-distribution estimates and those from the normal distribution as prior model. We can try other types of prior distributions as well, but for now I will halt with the normal and the t-distribution. Choosing appropriate priors is one of the hardest aspect of Bayesian Modeling, but we can get around that by having more data. As the amount of data the model learns from increases, the prior has less of an effect because each time the posterior is updated based on the new data. Essentially machine learning models perform inference with no priors, basing the final model entirely on the data. In the case of limited samples, Bayesian Inference can be a better method for building models because it provides a reasonable estimate in situations with few data points (as long as the prior is reasonable).

12 Conclusions

In this notebook we looked at using Bayesian Linear Regression to predict student performance based on five factors. Rather than specify probabilities for the Bayesian network which is basically impossible for continuous variables, we framed the problem as a machine learning task. In addition to the standard machine learning models that learn from observations, we also used Bayesian Linear Regression to create a model mapping the features (student characteristics) to the targets (final grade). The advantages of Bayesian Linear Regression are that if we use sensible priors, we can still get a decent estimate with few samples, and the final weights are not a single number, but a distribution componsed of every sample drawn during the sampling run. We can then make predictions using all the sampled weights to form a distribution of expected values rather than a single answer.

The Bayesian Linear Regression did not perform as well as the other methods in terms of the two metrics we choose. This might not be the ideal case for a Bayesian inference approach but we saw that Bayesian Linear Regression produced intuitive estimates for the model weights and gave predictions for new students that align with our expectations for the factors influencing student performance. To summarize, although Bayesian Linear Regression did not outperform the standard machine learning methods, it gave us a chance to learn another tool for use in evaluation and making sense of data. There are likely situations in which Bayesian inference is better suited than standard machine learning, and it is best to be prepared for those situations when we find them.