Jhirsc21

April 7, 2024

```
[1]: import warnings
  warnings.filterwarnings('ignore')

[2]: %matplotlib inline
```

1 Module 11 Lab - Model Evaluation

1.1 Directions

The due dates for each are indicated in the Syllabus and the course calendar. If anything is unclear, please email EN685.648@gmail.com the official email for the course or ask questions in the Lab discussion area on Blackboard.

The Labs also present technical material that augments the lectures and "book". You should read through the entire lab at the start of each module.

Please follow the directions and make sure you provide the requested output. Failure to do so may result in a lower grade even if the code is correct or even 0 points.

- 1. Show all work/steps/calculations using Code and Markdown cells.
- 2. Submit your notebook (.ipynb).
- 3. You may use any core Python libraries or Numpy/Scipy. Additionally, code from the Module notebooks and lectures is fair to use and modify. You may also consult Stackoverflow (SO). If you use something from SO, please place a comment with the URL to document the code.

```
[3]: import numpy as np
  import scipy.stats as stats
  import seaborn as sns
  import matplotlib.pyplot as plt
  import pandas as pd
  import random
  import patsy
  import sklearn.linear_model as linear
  import models

sns.set(style="whitegrid")
# load whatever other libraries you need including models.py
```

1.2 Model Evaluation and Improvement

As we saw in both the Linear Regression and Logistic Regression modules, there is a Statistician's view of Model Evaluation (and perhaps, Improvement) and a Machine Learning view of Model Evaluation and Improvement.

We'll be working with the insurance data.

1. Load the data, perform your transformations, and using the Bootstrap version of the Linear Regression function, estimate your final model from Lab 10 and show the Bootstrap results (You can also use the final model from the Solution if you like).

Here we load in the data and make sure it loads in correctly.

```
[4]: insurance = pd.read_csv("https://raw.githubusercontent.com/

-fundamentals-of-data-science/datasets/master/insurance.csv", header=0)
```

[5]: insurance.info()

<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1338 entries, 0 to 1337
Data columns (total 7 columns):

#	Column	Non-Null Count	Dtype
0	age	1338 non-null	int64
1	sex	1338 non-null	object
2	bmi	1338 non-null	float64
3	children	1338 non-null	int64
4	smoker	1338 non-null	object
5	region	1338 non-null	object
6	charges	1338 non-null	float64
dtype	es: float64	4(2), int64(2),	object(3)

memory usage: 73.3+ KB

[6]: insurance.head()

```
[6]:
                          bmi
                                children smoker
                 sex
                                                      region
                                                                    charges
        age
         19
              female
                       27.900
                                        0
                                                                16884.92400
     0
                                                   southwest
                                             yes
                       33.770
                                                                 1725.55230
     1
         18
                male
                                        1
                                              no
                                                   southeast
     2
         28
                male
                       33.000
                                        3
                                                                 4449.46200
                                                   southeast
     3
         33
                male
                       22.705
                                        0
                                                   northwest
                                                               21984.47061
     4
                                        0
         32
                male
                       28.880
                                                   northwest
                                                                 3866.85520
                                              no
```

It looks good to me. I'll be using the final model from the Lab 10 Solution. We had a model where charges was the target variable and our features included age_sq, male, bmi, smoke_yes; smoke_yes:bmi_above_30, and children.

Let's make sure we properly transform our variables correctly so we can use them in our model. Age is easy to square so we do that first, and can create the one hot encodings for our categorical variables sex -> male and smoker -> smokes_yes. Then we just apply a lambda function to get an encoding for bmi over 30 and we should be set.

Let's check our variables are in the dataframe

```
[8]: insurance.head()
```

False

True

True

```
[8]:
                              children smoker
        age
                sex
                         bmi
                                                   region
                                                                charges
                                                                         age_sq \
     0
         19
             female
                     27.900
                                     0
                                           yes
                                                southwest
                                                          16884.92400
                                                                            361
     1
         18
               male 33.770
                                     1
                                                southeast
                                                             1725.55230
                                                                            324
                                            no
     2
         28
               male 33.000
                                                            4449.46200
                                     3
                                                southeast
                                                                            784
                                            no
     3
         33
               male 22.705
                                     0
                                                northwest 21984.47061
                                                                           1089
     4
         32
               male 28.880
                                     0
                                                northwest
                                                             3866.85520
                                                                           1024
        female
                        smoke_no
                                  smoke_yes bmi_above_30
                 male
     0
          True
               False
                           False
                                       True
                                                         0
                                                         1
     1
         False
                 True
                            True
                                      False
     2
         False
                 True
                            True
                                      False
                                                         1
     3
         False
                 True
                            True
                                      False
                                                         0
```

Looks good to me. Now we can recreate this model and use bootstrap for linear regression from our models.py file.

0

```
[9]: model = "charges ~ age_sq + male + bmi + smoke_yes + smoke_yes:bmi +

⇔bmi_above_30 + smoke_yes:bmi_above_30 + children"

final = models.bootstrap_linear_regression(model, data=insurance)

models.describe_bootstrap_lr(final)
```

False

[9]: Model: charges \sim age_sq + male + bmi + smoke_yes + smoke_yes:bmi + bmi above 30 + smoke yes:bmi above 30 + children

			95% BCI	
Coefficients		Mean	${ m Lo}$	Hi
	β_0	2169.21	592.66	4036.82
age_sq	β_1	-517.49	-885.97	-13.15
male	β_2	1479.18	-3004.83	5717.87
bmi	β_3	3.34	3.17	3.58
$smoke_yes$	eta_4	-3.22	-73.32	60.87
$smoke_yes:bmi$	β_5	471.11	310.81	633.70
bmi_above_30	β_6	102.95	-1018.03	948.42
$smoke_yes:bmi_above_30$	β_7	15122.63	13655.35	17377.90
children	β_8	651.45	485.67	850.62
Metrics	Mean	Lo	Hi	
σ	4380.25	3910.25	4843.19	
R^2	0.87	0.84	0.90	

Note I include bmi_above_30 as a separate variable here because the bootstrap_linear_regression function was not working without including it in the model before the interaction term, though it's not necessary as we see the 95% BCI contains 0 and it may have an unexpected sign.

Here we have the estimates of the coefficients in the model for the bootstrap. We see an R^2 of 87% and a σ of 4380.25. Which is about a third of the original as we can see below

```
[10]: print('Original Std: ', '%.2f' % np.std(insurance['charges']))
print('Model Sigma: ', '%.2f' % final['sigma'])
```

Original Std: 12105.48 Model Sigma: 4380.25

2. Perform three rounds of 10-fold cross validation, estimating R^2 and σ each round. Using the results for the test data, calculate 95% Bootstrap estimates of the credible intervals for each. Comment on these intervals and the intervals from above. Are the average values different? Are the intervals different?

I'll be using the sklearn functions here to perform the cross validation, but note we could also make our own if we are inclined to do so. We need to first prepare our x's and y's in order to use the library properly.

```
[11]: from sklearn import datasets
```

```
[12]: X, y = datasets.load_iris(return_X_y=True)
```

Adding the interaction terms to the dataframe so we can select it easily in the next step.

```
[13]: insurance['interaction1'] = insurance['smoke_yes']*insurance['bmi'] insurance['interaction2'] = insurance['smoke_yes']*insurance['bmi_above_30']
```

Here is our 'x' data, we select all the observations with the features we want.

And here we simply select the target variable

```
[15]: y = insurance['charges'].values
```

Now we can create our cross validation using sklearn

```
[16]: from sklearn.model_selection import train_test_split, cross_val_score
```

We want to use a linear regression model

```
[17]: model = linear.LinearRegression()
```

Note we use negative mean squared error as our estimator, since this function uses a unified scoring API that maximizes the score, and we want to minimize our loss. This scoring simply returns the mse values multiplied by -1, and we can use the absolute value for our bootstrapping.

We can look at the R^2 and σ values as well here

```
R2 = 0.87
Sigma = 4344.29
```

An R^2 of about 86% and σ of 4344 for this model, pretty similar to what we found in question 1 (values of 87% and 4380, respectively).

We will perform the cross validation again for 2 more rounds, making sure we shuffle the data each time so we get different values for the MSE.

```
[19]: # this shuffles the observations in the dataframe
insurance = insurance.sample(frac=1).reset_index(drop=True)
```

We grab the features and target variables again and apply a 10 fold cross validation again and find the R^2 and σ each time. We will compare each round at the end.

R2 = 0.87Sigma = 4342.27

And one more time for round 3. Putting it all together

R2 = 0.86Sigma = 4367.18

Pretty similar values for each round of cross validation. Now we have 30 values of the mean squared error and can perform bootstrapping with our usual bootstrap_sample function from Lab 7.

```
[23]: mse_all = np.concatenate([scores1_mse, scores2_mse, scores3_mse])
    r2_all = np.concatenate([scores1_r2, scores2_r2, scores3_r2])
    sigma_all = np.concatenate([np.sqrt(scores1_mse), np.sqrt(scores2_mse),np.
    sqrt(scores3_mse)])
```

```
[24]: def bootstrap_sample( data, f, n=100):
    result = []
    m = len( data)
    for _ in range( n):
        sample = np.random.choice( data, len(data), replace=True)
        r = f( sample)
        result.append( r)
    return np.array( result)
```

```
[25]: posterior_mse = bootstrap_sample(mse_all, np.mean, 1000)
posterior_r2 = bootstrap_sample(r2_all, np.mean, 1000)
posterior_sigma = bootstrap_sample(sigma_all, np.mean, 1000)
```

We can look at a histogram of the posterior as well but I don't think it's necessary or interesting here. We can move on to looking at the 95% BCI

```
[26]: print( "95% BCI for mse theta:", stats.mstats.mquantiles(posterior_mse, [0.025, 0.00.975]))

print( "95% BCI for r2 theta:", stats.mstats.mquantiles(posterior_r2, [0.025, 0.0975]))

print( "95% BCI for sigma:", stats.mstats.mquantiles(posterior_sigma, [0.025, 0.0975]))
```

```
95% BCI for mse theta: [17589377.17136531 21033214.32871954]
95% BCI for r2 theta: [0.84841817 0.87979667]
95% BCI for sigma: [4146.19265574 4560.0842519]
```

We see for our R^2 we have a range of 0.848 to 0.879, compared to part 1 where the range was 0.84 to 0.90. We have a tighter range from the cross validation and bootstrapping. Our σ range here is 4146 to 4560, compared to part 1 of 3909 to 4885, roughly. Again we see a bit of a tighter range with the cross validation process.

```
[28]: from tabulate import tabulate
```

Here is a simple table to compare each cross validation round with our original model.

As we already saw, the average values for these statistics are pretty much the same between part 1 and the cross validation techniques, with the σ for part 1 being slightly higher. Overall however

we get very similar results.

3. Using Learning Curves and σ as your evaluation metric determine if more data will improve the estimation of the model.

For this part I'll be using the code from *Fundamentals*, page 878 in order to calculate our learning curves and standard error.

```
[30]: import collections
      from patsy.highlevel import dmatrices
[31]: def sse(results):
          errors = results['residuals']
          n = len(errors)
          squared error = np.sum([e**2 for e in errors])
          return np.sqrt((1.0/n)*squared_error)
[32]: def chunk(xs, n):
          k,m = divmod(len(xs), n)
          return [xs[i*k + min(i,m):(i+1)*k + min(i+1, m)] for i in range(n)]
[33]: def data_collection():
          result = dict()
          result['train'] = collections.defaultdict(list)
          result['test'] = collections.defaultdict(list)
          return result
[34]: def learning_curves(algorithm, formula, data, evaluate, fold_count=10,
                          repetitions=3, increment=1):
          indices = list(range(len(data)))
          results = data_collection()
          for _ in range(repetitions):
              random.shuffle(indices)
              folds = chunk(indices, fold_count)
              for fold in folds:
                  test_data = data.iloc[fold]
                  train indices = [idx for idx in indices if idx not in fold]
                  train_data = data.iloc[train_indices]
                  for i in list(range(increment, 100, increment)) + [100]:
                      train_chunk_size = int(np.ceil((i/100)*len(train_indices)))
                      train_data_chunk = data.iloc[train_indices[0:train_chunk_size]]
                      result = algorithm(formula, data=train_data_chunk)
                      model = result['model']
                      y, X = dmatrices(formula, train_data_chunk,_
       →return_type='matrix')
                      result = models.summarize(formula, X, y, model)
                      metric = evaluate(result)
                      results['train'][i].append(metric)
```

```
y, X = dmatrices(formula, test_data, return_type='matrix')
    result = models.summarize(formula, X, y, model)
    metric = evaluate(result)
    results['test'][i].append(metric)

statistics = {}
for k, v in results['train'].items():
    statistics[k] = (np.mean(v), np.std(v))
results['train'] = statistics

statistics = {}
for k, v in results['test'].items():
    statistics[k] = (np.mean(v), np.std(v))
results['test'] = statistics
return results
```

Now we can get results for our learning curves using standard error (sse) and a linear regression model for our data.

```
[35]: model = "charges ~ age_sq + male + bmi + smoke_yes + smoke_yes:bmi +

⇔bmi_above_30 + smoke_yes:bmi_above_30 + children"

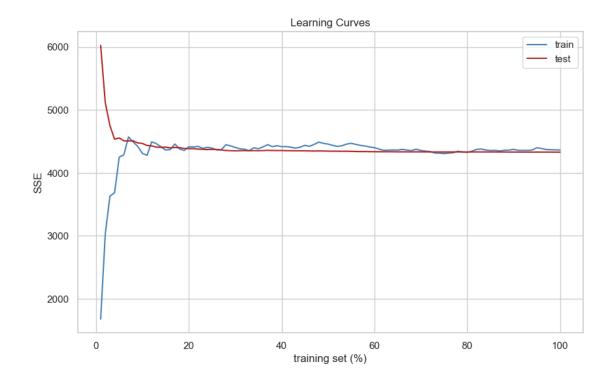
results = learning_curves(models.linear_regression, model, insurance, sse)
```

Using the functions from *Fundamentals*, page 880 and on, we can plot our results for the training data and test data to compare.

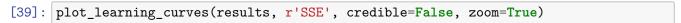
```
[36]: def results_to_curves(curve, results):
    all_statistics = results[curve]
    keys = list(all_statistics.keys())
    keys.sort()
    mean = []
    upper = []
    lower = []
    for k in keys:
        m,s = all_statistics[k]
        mean.append(m)
        upper.append(m + 2 * s)
        lower.append(m - 2 * s)
    return keys, lower, mean, upper
```

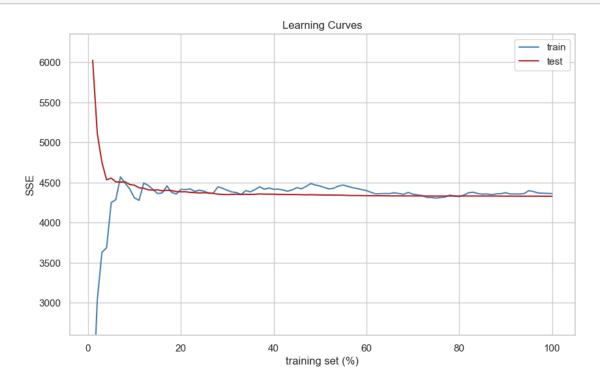
```
xs, train_lower, train_mean, train_upper = results_to_curves('train',_
⇔results)
  _, test_lower, test_mean, test_upper = results_to_curves('test', results)
  axes.plot(xs, train_mean, color='steelblue', label='train')
  axes.plot(xs, test mean, color='firebrick', label='test')
  if credible:
       axes.fill_between(xs, train_upper, train_lower, color='steelblue', u
\rightarrowalpha=0.25)
       axes.fill_between(xs, test_upper, test_lower, color='firebrick',__
\rightarrowalpha=0.25)
  if desired:
       if type(desired) is tuple:
           axes.axhline((desired[0] + desired[1]) / 2.0, color='gold',__
⇔label='desired')
           axes.fill_between(xs, desired[1], desired[0], color='gold', alpha=0.
⇒25)
       else:
           axes.axhline(desired, color='gold', label='desired')
  axes.legend()
  axes.set_xlabel('training set (%)')
  axes.set_ylabel(metric)
  axes.set_title('Learning Curves')
  if zoom:
       y_lower = int(0.9*np.amin([train_lower[-1], test_lower[-1]]))
      y_upper = int(1.1*np.amax([train_upper[-1], test_upper[-1]]))
      axes.set_ylim((y_lower, y_upper))
  plt.show()
  plt.close()
```

```
[38]: plot_learning_curves(results, r'SSE', credible=False)
```



We see here that the training and test curves start to converge around 30% of the training set, and the SSE is around 4400-4500. Let's zoom in for a closer look.





We can see the SSE around the 30% and higher of the training data is definitely around the 4400 mark. This is slightly higher but still consistent with the SSE results we found for parts 1 and 2. I don't believe getting more data will help, as we do have a pretty good convergence by the time we evaluate 100% of the data in training and test sets.

4. It was shown that age_sq improved the performance of the model. Perhaps a different polynomial would have been better. Generate Validation Curves for age_n where n = [1.5, 1.6, 1.7, 1.8, 1.9, 2.0, 2.1, 2.2, 2.3, 2.4, 2.5] and select the best transformation.

In order to get our validation curves, I will use the functions from *Fundamentals*, page 887 and pretend I know what's going on.

```
[40]: def validation_curves(algorithm, formulas, data, values, evaluate,
       →fold_count=10, repetitions=3, increment=1):
          indices = list(range(len(data)))
          results = data_collection()
          for in range(repetitions):
              random.shuffle(indices)
              folds = chunk(indices, fold count)
              for fold in folds:
                  test_data = data.iloc[fold]
                  train_indices = [idx for idx in indices if idx not in fold]
                  train_data = data.iloc[train_indices]
                  for i, p in enumerate(zip(formulas, values)):
                      f, v = p
                      result = algorithm(f, train_data, v)
                      model = result['model']
                      y, X = dmatrices(f, train_data, return_type='matrix')
                      result = models.summarize(f, X, y, model)
                      metric = evaluate(result)
                      results['train'][i].append(metric)
                      y, X = dmatrices(f, test_data, return_type='matrix')
                      result = models.summarize(f, X, y, model)
                      metric = evaluate(result)
                      results['test'][i].append(metric)
          statistics = {}
          for k, v in results['train'].items():
              statistics[k] = (np.mean(v), np.std(v))
          results['train'] = statistics
          statistics = {}
          for k, v in results['test'].items():
              statistics[k] = (np.mean(v), np.std(v))
```

```
results['test'] = statistics
return results
```

Let's try the difference values for age_sq

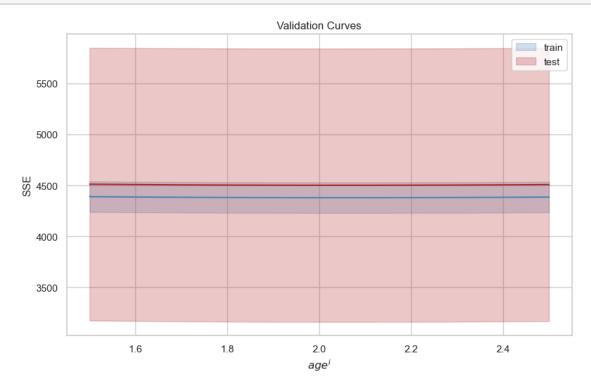
Now we can look at some plots

```
[42]: def plot_validation_curves(results, metric, parameter, values, zoom=False):
          figure = plt.figure(figsize=(10,6))
          axes = figure.add subplot(1,1,1)
          xs, train_lower, train_mean, train_upper = results_to_curves('train', _
       ⇔results)
          _, test_lower, test_mean, test_upper = results_to_curves('test', results)
          axes.plot(values, train mean, color='steelblue')
          axes.fill_between(values, train_upper, train_lower, color='steelblue',_
       →alpha=0.25, label='train')
          axes.plot(values, test_mean, color='firebrick')
          axes.fill_between(values, test_upper, test_lower, color='firebrick',_
       ⇒alpha=0.25, label='test')
          axes.legend()
          axes.set_xlabel(parameter)
          axes.set ylabel(metric)
          axes.set_title('Validation Curves')
```

```
if zoom:
    y_lower = int(0.9*np.amin([train_lower[-1], test_lower[-1]]))
    y_upper = int(1.1*np.amax([train_upper[-1], test_upper[-1]]))
    axes.set_ylim((y_lower, y_upper))

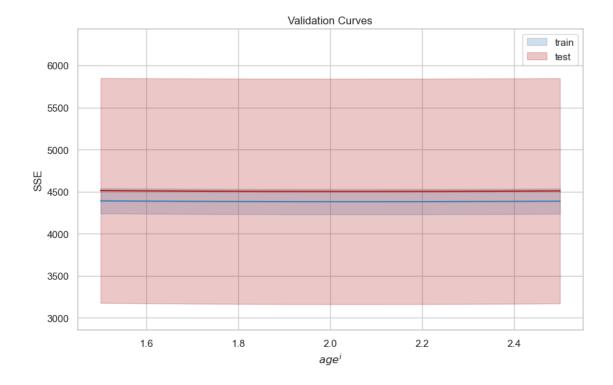
plt.show()
plt.close()
```

```
[43]: plot_validation_curves(result, 'SSE', r'$age^i$', values)
```



Hmm we don't see much of a difference here. Of course our values for the age parameter are not too different from each other, but we might still expect a notable difference between say 1.5 and 2.5. Let's try zooming to see if that makes a difference.

```
[44]: plot_validation_curves(result, 'SSE', r'$age^i$', values, zoom=True)
```



Pretty much the same. It doesn't seem like changing these values for the age variable makes much of a difference, but maybe they are just too close together. We might also try values of 0.5 and 4 to see how they look, but for brevity I will not include it here. There may just be too many other variables in the model so that slightly changing age here does not make as much of a difference as we would like to see.

5. Using Ridge Regression to estimate a model for the insurance data. Compare it with your final Linear Regression model. (If you get far ahead, you may need to write your own function. Here are the sklearn docs: http://scikit-learn.org/stable/modules/linear model.html)

We can use the sklearn Ridge class to fit our model.

[45]: Coefficients 2301.246891 intercept age_sq 3.344330 male -517.194198 bmi -8.909586 smoke_yes 831.997102 smoke_yes:bmi 499.230868 bmi_above_30 184.444723 smoke_yes:bmi_above_30 14708.020001 children 651.354969

Here we have the coefficients for our ridge regression. Below is our final linear regression model from part 1 as a reminder of the coefficients.

```
[46]: reg.score(x, y)
```

[46]: 0.8699358637434325

We can also see our R^2 value from the ridge regression is about 87%, nearly identical to our final linear model regression model. The coefficients are fairly similar between models, with the exceptions of age_sq, male, and smoke_yes.

```
[47]: models.describe_bootstrap_lr(final)
```

Model: charges \sim age_sq + male + bmi + smoke_yes + smoke_yes:bmi + bmi_above_30 + smoke_yes:bmi_above_30 + children

			95% BCI	
Coefficients		Mean	${f Lo}$	${ m Hi}$
	β_0	2169.21	592.66	4036.82
age_sq	β_1	-517.49	-885.97	-13.15
male	eta_2	1479.18	-3004.83	5717.87
bmi	β_3	3.34	3.17	3.58
$smoke_yes$	eta_4	-3.22	-73.32	60.87
$smoke_yes:bmi$	β_5	471.11	310.81	633.70
bmi_above_30	β_6	102.95	-1018.03	948.42
$smoke_yes:bmi_above_30$	β_7	15122.63	13655.35	17377.90
children	β_8	651.45	485.67	850.62
Metrics	Mean	${f Lo}$	${ m Hi}$	
σ	4380.25	3910.25	4843.19	
R^2	0.87	0.84	0.90	

Based on what we've done for each part, it seems that the final linear regression model is probably

sufficient for our needs. We found that adding more data would not significantly improve the model through learning curves, and performed cross validation with bootstrapping, which still gave similar results as our final linear model.

With Ridge Regression, we also found similar results, and saw that with our validation curves, changing the polynomial for our age variable did not significantly change our model, likely because we have too many other coefficients.