cs109a_hw3_209_joshua_feldman

October 2, 2018

1 CS109A Introduction to Data Science:

1.1 Homework 3 AC 209 : From MLE to AIC

Harvard University Fall 2018 Instructors: Pavlos Protopapas, Kevin Rader

```
In [27]: #RUN THIS CELL
         import requests
         from IPython.core.display import HTML
         styles = requests.get("https://raw.githubusercontent.com/Harvard-IACS/2018-CS109A/mas
         HTML(styles)


        ---------------------------------------------------------------------------

        gaierror                                  Traceback (most recent call last)

        ~/anaconda3/envs/py36/lib/python3.6/site-packages/urllib3/connection.py in _new_conn(se
        170             conn = connection.create_connection(
    --> 171                 (self._dns_host, self.port), self.timeout, **extra_kw)
        172


        ~/anaconda3/envs/py36/lib/python3.6/site-packages/urllib3/util/connection.py in create_
         55
    ---> 56     for res in socket.getaddrinfo(host, port, family, socket.SOCK_STREAM):
         57         af, socktype, proto, canonname, sa = res


        ~/anaconda3/envs/py36/lib/python3.6/socket.py in getaddrinfo(host, port, family, type,
        744     addrlist = []
    --> 745     for res in _socket.getaddrinfo(host, port, family, type, proto, flags):
        746         af, socktype, proto, canonname, sa = res


        gaierror: [Errno 8] nodename nor servname provided, or not known
```

During handling of the above exception, another exception occurred:

```
    NewConnectionError                        Traceback (most recent call last)

    ~/anaconda3/envs/py36/lib/python3.6/site-packages/urllib3/connectionpool.py in urlopen
    599                                                       body=body, headers=headers,
--> 600                                                       chunked=chunked)
    601


    ~/anaconda3/envs/py36/lib/python3.6/site-packages/urllib3/connectionpool.py in _make_re
    342         try:
--> 343             self._validate_conn(conn)
    344         except (SocketTimeout, BaseSSLError) as e:


    ~/anaconda3/envs/py36/lib/python3.6/site-packages/urllib3/connectionpool.py in _valida
    848         if not getattr(conn, 'sock', None):  # AppEngine might not have  `.sock`
--> 849             conn.connect()
    850


    ~/anaconda3/envs/py36/lib/python3.6/site-packages/urllib3/connection.py in connect(sel
    313         # Add certificate verification
--> 314         conn = self._new_conn()
    315


    ~/anaconda3/envs/py36/lib/python3.6/site-packages/urllib3/connection.py in _new_conn(se
    179             raise NewConnectionError(
--> 180                 self, "Failed to establish a new connection: %s" % e)
    181


    NewConnectionError: <urllib3.connection.VerifiedHTTPSConnection object at 0x1c19484cc0
```

During handling of the above exception, another exception occurred:

```
    MaxRetryError                             Traceback (most recent call last)

    ~/anaconda3/envs/py36/lib/python3.6/site-packages/requests/adapters.py in send(self, re
    444                     retries=self.max_retries,
--> 445                     timeout=timeout
    446                 )
```

```
    ~/anaconda3/envs/py36/lib/python3.6/site-packages/urllib3/connectionpool.py in urlopen
    637             retries = retries.increment(method, url, error=e, _pool=self,
--> 638                                             _stacktrace=sys.exc_info()[2])
    639             retries.sleep()


    ~/anaconda3/envs/py36/lib/python3.6/site-packages/urllib3/util/retry.py in increment(se
    397         if new_retry.is_exhausted():
--> 398             raise MaxRetryError(_pool, url, error or ResponseError(cause))
    399


    MaxRetryError: HTTPSConnectionPool(host='raw.githubusercontent.com', port=443): Max re


During handling of the above exception, another exception occurred:


    ConnectionError                           Traceback (most recent call last)

    <ipython-input-27-7b90700e881a> in <module>()
      2 import requests
      3 from IPython.core.display import HTML
----> 4 styles = requests.get("https://raw.githubusercontent.com/Harvard-IACS/2018-CS109A/m
      5 HTML(styles)


    ~/anaconda3/envs/py36/lib/python3.6/site-packages/requests/api.py in get(url, params, *
     70
     71     kwargs.setdefault('allow_redirects', True)
---> 72     return request('get', url, params=params, **kwargs)
     73
     74


    ~/anaconda3/envs/py36/lib/python3.6/site-packages/requests/api.py in request(method, ur
     56     # cases, and look like a memory leak in others.
     57     with sessions.Session() as session:
---> 58         return session.request(method=method, url=url, **kwargs)
     59
     60


    ~/anaconda3/envs/py36/lib/python3.6/site-packages/requests/sessions.py in request(self
    510         }
    511         send_kwargs.update(settings)
```

```
--> 512         resp = self.send(prep, **send_kwargs)
    513
    514         return resp


    ~/anaconda3/envs/py36/lib/python3.6/site-packages/requests/sessions.py in send(self, r
    620
    621         # Send the request
--> 622         r = adapter.send(request, **kwargs)
    623
    624         # Total elapsed time of the request (approximately)


    ~/anaconda3/envs/py36/lib/python3.6/site-packages/requests/adapters.py in send(self, r
    511                 raise SSLError(e, request=request)
    512
--> 513             raise ConnectionError(e, request=request)
    514
    515         except ClosedPoolError as e:


    ConnectionError: HTTPSConnectionPool(host='raw.githubusercontent.com', port=443): Max r
```

In [28]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from scipy.stats import t
from scipy.optimize import minimize

from statsmodels.api import OLS
import statsmodels.api as sm
from scipy.stats import norm
%matplotlib inline
```

Question 7: Student's t MLE

7.1 Fit a simple linear regression model using Maximum Likelihood Estimation on the data provided in `data/beerdata.csv`. Consider two statistical models the for noise: a) Normal and b) Student's t-distribution with $\nu = 5$ and scale factor $\sigma = \sqrt{3/5}$.

7.2 Compare the two models performances (visualize the prediction lines and estimate the KL divergence between the data and each model) and comment why it is perhaps appropriate to use the Student's t-distribution instead of the Normal.

Hints: 1. Use the probability density function for the Student's t distribution with location t, ν degrees of freedom and scale factor σ. 2. If the MLE regression coefficients cannot be derived analytically consider numerical methods. 3. For *convenience*, you can use sklearn or statsmodel for the Normal case.

1.1.1 Answers

7.1 Fit a simple linear regression model using Maximum Likelihood Estimation on the data provided in `data/beerdata.csv`. Consider two statistical models the for noise: a) Normal and b) Student's t-distribution with $\nu = 5$ and scale factor $\sigma = \sqrt{3/5}$.

your answer here

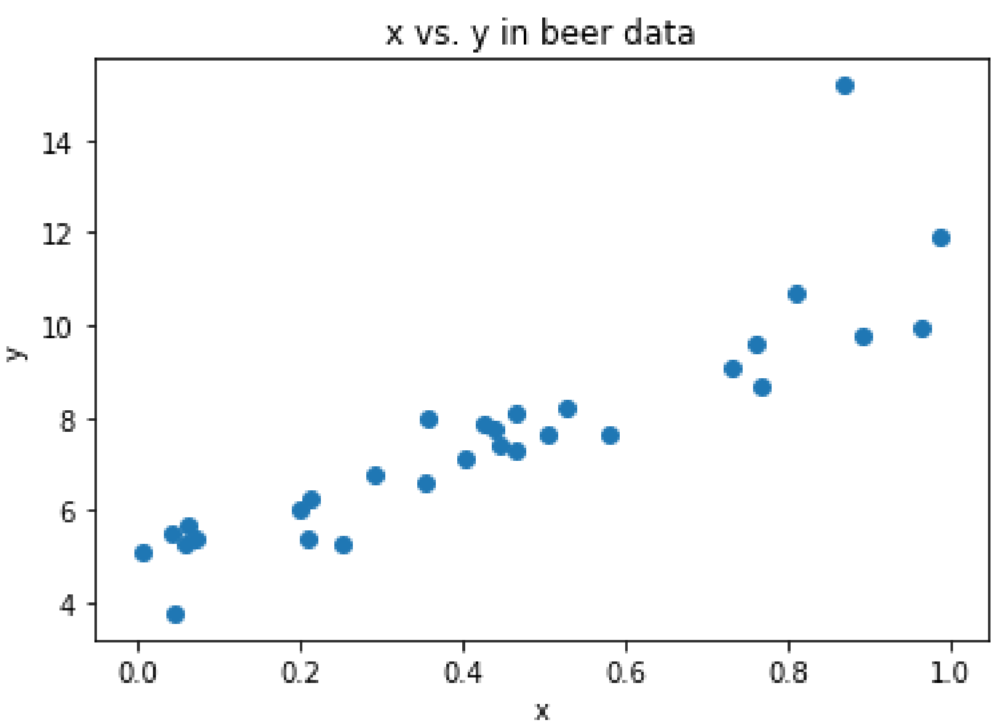
```
In [29]: #Read and show the data
         # your code here
         beer_df = pd.read_csv('./data/beerdata.csv').drop(columns=['Unnamed: 0'])
         beer_df.head()
```

Out[29]:

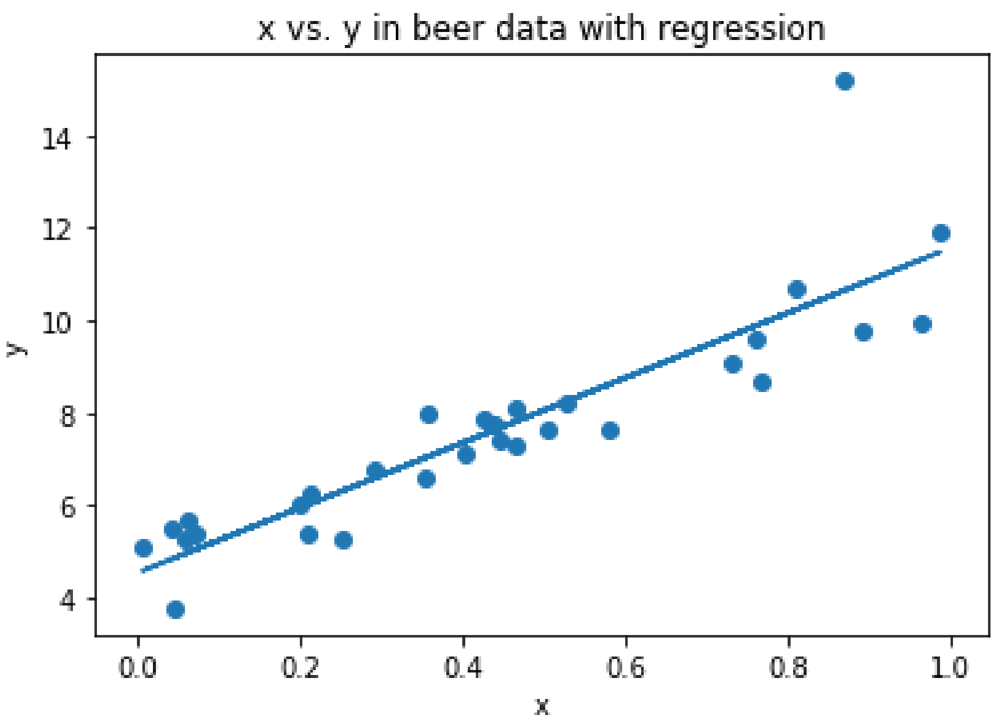
	x	y
0	0.760083	9.616565
1	0.766794	8.652492
2	0.504173	7.653462
3	0.357411	7.984081
4	0.730932	9.080448

```
In [30]: #### Plot the data
         # your code here
         plt.scatter(beer_df.x, beer_df.y)
         plt.xlabel('x')
         plt.ylabel('y')
         plt.title("x vs. y in beer data")
```

```
Out[30]: Text(0.5,1,'x vs. y in beer data')
```



```
In [31]: #### Generate the ordinary least squares model (OLS)
         # your code here
         ols_model = OLS(beer_df.y, sm.add_constant(beer_df.x)).fit()

In [32]: #### Plot the data along with OLS fit line
         # your code here
         plt.scatter(beer_df.x, beer_df.y)
         plt.plot(beer_df.x, ols_model.predict(sm.add_constant(beer_df.x)))
         plt.xlabel('x')
         plt.ylabel('y')
         plt.title("x vs. y in beer data with regression")

Out[32]: Text(0.5,1,'x vs. y in beer data with regression')
```




```
In [33]: #### LET'S MAKE THE REGRESSION MODEL WITH t-Students distribution
         # your code here
         class StudentRegression(object):
             def __init__(self, df, sigma, X, y):
                 self.params = {'df' : df,'sigma' : sigma}
                 self.X = X.values.reshape(-1,1)
                 self.n = self.X.shape[0]
```

```
            self.X = np.append(self.X, np.ones(self.n).reshape(self.n,1), axis = 1)
            self.y = y.values.reshape(-1,1)

        def get_params(self, k):
            return self.params[k]

        def set_params(self, **kwargs):
            for k,v in kwargs.items():
                self.params[k] = v

        def fit(self):
            logpdf = lambda x: t.logpdf(x, self.params['df'], loc=0, scale=self.params['s
            neg_log_likelihood = lambda coef: -np.sum(logpdf(self.X.dot(coef).reshape(-1,

            #calculate coefficients
            coef_init = np.array([7,4]).reshape(-1,1)
            coef = minimize(neg_log_likelihood, coef_init, method='Nelder-Mead')
            self.params['coef'] = coef.x

        def predict(self, X_pred):
            x = X_pred.values.reshape(-1,1)
            x = np.append(x, np.ones(x.shape[0]).reshape(-1,1), axis=1)
            return x.dot(self.params['coef'])

        def score(self, X, y):
            # your code
            SST = np.sum((y-np.mean(y))**2)
            SSE = np.sum((y-self.predict(X))**2)
            return 1 - SSE/SST
```

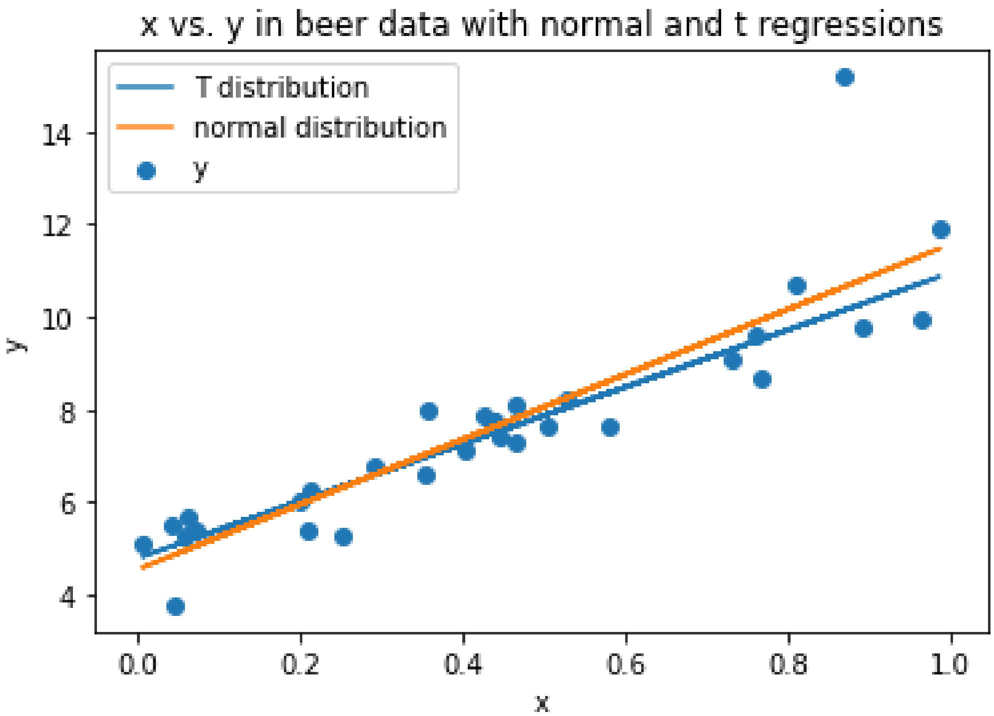
In [34]:
```
t_model = StudentRegression(5, np.sqrt(3/5), beer_df.x, beer_df.y)
t_model.fit()
t_model.params
```

Out[34]:
```
{'df': 5, 'sigma': 0.7745966692414834, 'coef': array([6.17291817, 4.7738314 ])}
```

7.2 Compare the two models performances (visualize the prediction lines and estimate the KL divergence between the data and each model) and comment why it is perhaps appropriate to use the Student's t-distribution instead of the Normal.

your answer here

In [35]:
```
plt.scatter(beer_df.x, beer_df.y)
plt.plot(beer_df.x, t_model.predict(beer_df.x),label ="T distribution")
plt.plot(beer_df.x, ols_model.predict(sm.add_constant(beer_df.x)),label ="normal dist
plt.xlabel('x')
plt.ylabel('y')
plt.legend()
plt.title("x vs. y in beer data with normal and t regressions")
plt.show()
```




```
In [37]: # your code here
         resid_t = beer_df.y - t_model.predict(beer_df.x)
         resid_norm = beer_df.y - ols_model.predict(sm.add_constant(beer_df.x))

         pdf_t = lambda x : t.pdf(x, df = 5, loc = 0, scale = np.sqrt(3/5))
         pdf_norm = lambda x : norm.pdf(x, scale = np.std(resid_norm))

         print("KL divergence for normal distribution minus KL for t-distribution:", np.mean(np
```

```
KL divergence for normal distribution minus KL for t-distribution: 0.23090166134812778
```

your answer here

Visually inspecting the plot above suggests that the t-distribution fits our data better. This is because the tails of t-distributions are larger so linear regressions that assume a t-distribution are less sensitive to outliers.

To formalize this, consider the KL divergences. Let p_{data} be the empirical distribution estimating the data generating process, p_{norm} be the normal distribution we fit in our regression, and p_t be the t distribtion we also fit via regression.

$$D(p_{data}, p_{norm}) - D(p_{data}, p_t) = \frac{1}{N} \sum_i \left(\frac{p_t(y_i)}{p_{norm}(y_i)} \right) > 0$$

Hence, the KL divergence between our empirical distribution and the normal distribution is greater than the KL divergence between the empirical distribution and the t distribution. Assuming a t distribution for our data is less "surprising", meaning that it is a better fit

Question 8: Akaike Information Criterion (AIC)

Perform a simple numerical experiment to understand and demonstrate the AIC by using the given `generate_data` function to generate your data.

8.1 Generate data for different number of parameters k, in the range 1 to 10. For each of the six models generate 1000 training and 1000 testing datasets with each one containing $n = 50$ observations.

8.2 Use the training set to estimate the OLS coefficients and calculate the predicted values, $\hat{y}_{tr}$, on the training set and the log-likelihood. Use the OLS coefficients to calculate the predicted values for the testing set, $\hat{y}_{te}$, and the associated log-likelihood.

8.3 For each k compute the average and standard deviation of the log-likelihoods across the 1000 simulations. Plot the average log-likelihoods (with error bars) and the average AIC as function of k, the number of parameters. What is the best k based on AIC?

8.4 Verify the results in 8.3 by plotting the average log-likelihoods for each of the training and testing datasets as a function of k. What is the best k based on this plot?

Comment: 1. The function "generate_data" uses an interesting trick to generate data directly using the regression coefficients as proxies for the correlations with the response variable. It generates data from a Normal distribution, hence $y_i \sim \mathcal{N}(\mu_i = 0.15x_{1,i} - 0.4x_{2,i}, \sigma^2 = 1)$.

```
In [38]: def generate_data(N,k,beta=[0.15 , -0.4]):

             ## N: The number of observations
             ## k: The number of parameters
             ## beta is the weights vector for the covariates x1, x2
             ##
             ## Make d_min be greater or equal to k
             n_dim = 1+len(beta)
             if (n_dim <= k):
                 n_dim = k

             Rho = np.eye(n_dim)

             # Add beta in the first row or Rho
             for i,r in enumerate(beta):
                 Rho[0,i+1] = r

             index_lower = np.tril_indices(n_dim, -1)

             Rho[index_lower] = Rho.T[index_lower]
             mean = n_dim * [0.]
             Xtrain = np.random.multivariate_normal(mean, Rho, size=N)
             Xtest = np.random.multivariate_normal(mean, Rho, size=N)
             ytrain = Xtrain[:,0].copy()
             Xtrain[:,0]=1.
             ytest = Xtest[:,0].copy()
             Xtest[:,0]=1.
             return Xtrain[:,:k], ytrain, Xtest[:,:k], ytest
```

1.1.2 Answers

8.1 Generate data for different number of parameters k, in the range 1 to 10. For each of the ten models generate 1000 training and 1000 testing datasets with each one containing $n = 50$ observations.

```
In [39]: #### Be familiar with the generated data by printing them:
         # your code here
         for d in generate_data(10,2):
             print(d)
             print('----------------')
```

```
[[ 1.         -0.7767165 ]
 [ 1.          0.18501063]
 [ 1.         -0.73732799]
 [ 1.         -0.25335297]
 [ 1.          1.1376084 ]
 [ 1.          0.22246277]
 [ 1.          0.34706842]
 [ 1.         -0.34763334]
 [ 1.         -0.48151691]
 [ 1.          0.16379733]]
----------------
[-1.21968    -0.10755208  0.5450195  -0.79343618 -0.02283883 -0.42269615
 -0.53257513  0.38050016  0.32485441 -2.58128748]
----------------
[[ 1.          1.0810378 ]
 [ 1.         -1.34142167]
 [ 1.          1.51782813]
 [ 1.         -0.770207  ]
 [ 1.          1.48409741]
 [ 1.          0.03071772]
 [ 1.          0.30117271]
 [ 1.         -1.20770116]
 [ 1.         -0.1563523 ]
 [ 1.          0.02415695]]
----------------
[-0.19767861 -1.90577327  1.05153771  1.60530385  1.17492306 -2.63740153
 -0.42915273  1.31277591 -0.04681281  0.62936748]
----------------
```

```
In [40]: data_all = {}
         for k in range(1,11):
             data_all[k] = [generate_data(50,k) for _ in range(1000)]
```

8.2 Use the training set to estimate the OLS coefficients and calculate the predicted values, $\hat{y}_{tr}$, on the training set and the associated log-likelihood. Use the OLS coefficients to calculate the predicted values for the testing set, $\hat{y}_{te}$, and the associated log-likelihood.

```
In [41]: def log_likelihood(y,y_pred):
             resid = y-y_pred
             return np.sum(norm.logpdf(resid))
```

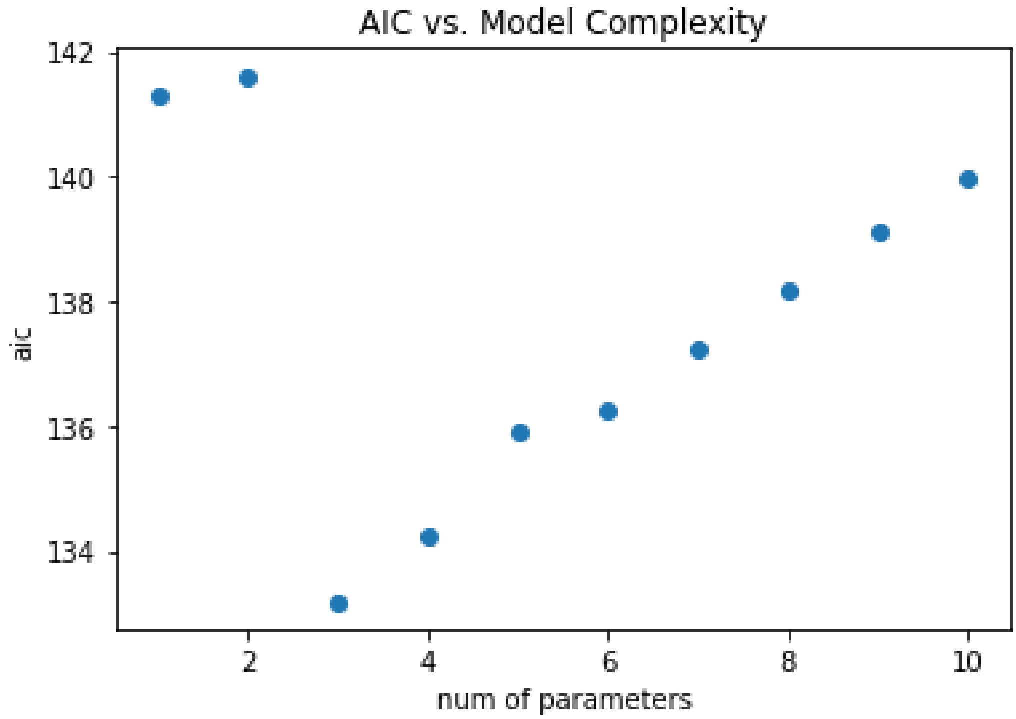
```
In [42]: # your code here
         outputs = {}
         for k in data_all:

             # initialize output
             outputs[k] = {}
             outputs[k]['y_train_pred'] = []
             outputs[k]['y_train_log_likelihood'] = []
             outputs[k]['y_test_pred'] = []
             outputs[k]['y_test_log_likelihood'] = []
             outputs[k]['aic'] = []

             for data in data_all[k]:
                 # fit model
                 model = OLS(data[1],data[0]).fit()

                 #record aic
                 outputs[k]['aic'].append(model.aic)

                 # make predictions on train set
                 y_train_pred = model.predict(data[0])
                 outputs[k]['y_train_pred'].append(y_train_pred)
                 outputs[k]['y_train_log_likelihood'].append(log_likelihood(data[1],y_train_pr

                 # make predictions on test set
                 y_test_pred = model.predict(data[2])
                 outputs[k]['y_test_pred'].append(y_test_pred)
                 outputs[k]['y_test_log_likelihood'].append(log_likelihood(data[3],y_test_pred
```

8.3 For each k compute the average and standard deviation of the log-likelihoods across the 2000 simulations. Plot the average log-likelihoods (with error bars) and the average AIC as function of k, the number of parameters. What is the best k based on AIC?

```
In [43]: # your code here
         average_likelihoods_train = [np.mean(outputs[k]['y_train_log_likelihood']) for k in ou
         std_likelihoods_train = [np.std(outputs[k]['y_train_log_likelihood']) for k in outputs
         average_likelihoods_test = [np.mean(outputs[k]['y_test_log_likelihood']) for k in outp
         std_likelihoods_test = [np.std(outputs[k]['y_test_log_likelihood']) for k in outputs]
         average_aic_train = [np.mean(outputs[k]['aic']) for k in outputs]
```

```
In [46]: plt.scatter(data_all.keys(), average_aic_train)
         plt.xlabel('num of parameters')
         plt.ylabel('aic')
         plt.title('AIC vs. Model Complexity')
```

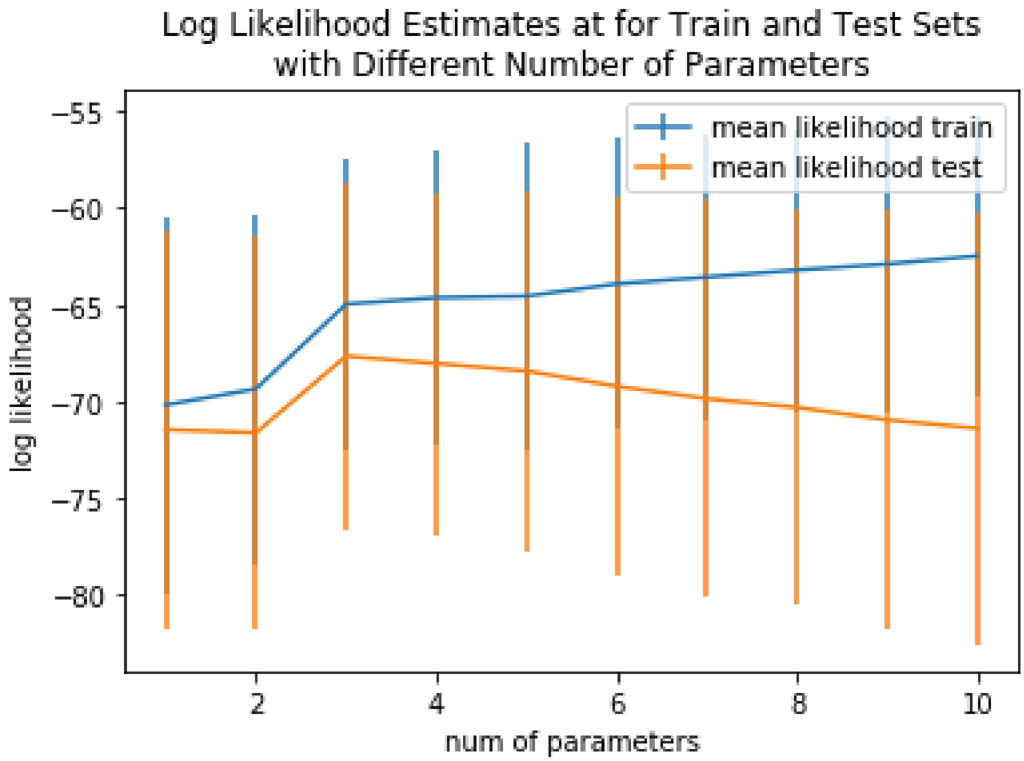
Out[46]: Text(0.5,1,'AIC vs. Model Complexity')



The best k based on aic is 3

8.4 Verify the results in 8.3 by plotting the average log-likelihoods for each of the training and testing datasets as a function of k. What is the best k based on this plot?

In [45]:
```
#### Plot the log-likelihood for the traing and testing:
# your code here
#plt.scatter(data_all.keys(),average_aic,label='mean aic')
plt.errorbar(data_all.keys(), average_likelihoods_train,
             yerr=np.array(std_likelihoods_train)*1.96,
             label = 'mean likelihood train')
plt.errorbar(data_all.keys(), average_likelihoods_test,
             yerr=np.array(std_likelihoods_test)*1.96,
             label = 'mean likelihood test')

plt.xlabel('num of parameters')
plt.ylabel('log likelihood')
plt.title('Log Likelihood Estimates at for Train and Test Sets\n with Different Numbe
plt.legend()
plt.show()
```



The best validation likelihood is for k=3, which confirms the result provided by analyzing the AIC.