In [1]:
```
import numpy as np
from numpy import linalg as LA
import pandas as pd
from IPython.display import display, Math
from scipy.spatial import distance
import matplotlib.pyplot as plt
%matplotlib inline
```

In [2]:
```
# Best practice source:
# https://numpy.org/doc/stable/reference/random/generated/numpy.random.seed.h
from numpy.random import MT19937
from numpy.random import RandomState, SeedSequence
rs = RandomState(MT19937(SeedSequence(72730)))
```

In [3]:
```
p = 5
rho = .8
Sigma = np.full((p, p), rho)
np.fill_diagonal(Sigma, 1)
print(Sigma)
```

```
[[1.  0.8 0.8 0.8 0.8]
 [0.8 1.  0.8 0.8 0.8]
 [0.8 0.8 1.  0.8 0.8]
 [0.8 0.8 0.8 1.  0.8]
 [0.8 0.8 0.8 0.8 1. ]]
```

A) The marginal distribution of (Y_1, Y_2) is MVN with $\mu = (0, 0)'$ and $\Sigma =$

In [4]:
```
print(Sigma[:2, :2])
```

```
[[1.  0.8]
 [0.8 1. ]]
```

B) The conditional distribution of $(Y_1, Y_2)|Y_3, Y_4, Y_5$ is MVN. We calculate the mean $\bar\mu$ and covariance matrix $\bar\Sigma$ of this distribution below:

In [5]:
```
mu1 = np.array([0, 0])
mu2 = np.array([0, 0, 0])
givens = np.array([0.23, -0.65, -0.3])
sig22inv = LA.inv(Sigma[-3:, -3:])
mubar = mu1 + LA.multi_dot([Sigma[:2, -3:], sig22inv, givens])
display(Math(r'\bar\mu :'))
print(mubar)
sigbar = Sigma[:2, :2] - LA.multi_dot([Sigma[:2, -3:], sig22inv, Sigma[-3:, :
display(Math(r'\bar\Sigma :'))
print(sigbar)
```

$\displaystyle \bar\mu :$

```
[-0.22153846 -0.22153846]
```

$\displaystyle \bar\Sigma :$

```
[[0.26153846 0.06153846]
 [0.06153846 0.26153846]]
```

C) The L in $\Sigma = LL'$ comes from the Cholesky decomposition of Σ. It is one varaition on the square root of Σ. In this example, L is:

In [6]:
```
choleskyL = LA.cholesky(Sigma)
print(choleskyL)
```

```
[[1.         0.         0.         0.         0.        ]
 [0.8        0.6        0.         0.         0.        ]
 [0.8        0.26666667 0.53748385 0.         0.        ]
 [0.8        0.26666667 0.16537965 0.51140831 0.        ]
 [0.8        0.26666667 0.16537965 0.12033137 0.49705012]]
```

D) L^{-1} is:

In [7]:
```
print(LA.inv(choleskyL))
```

```
[[ 1.          0.          0.          0.          0.        ]
 [-1.33333333  1.66666667  0.          0.          0.        ]
 [-0.82689823 -0.82689823  1.86052102  0.          0.        ]
 [-0.60165684 -0.60165684 -0.60165684  1.95538472  0.        ]
 [-0.47338107 -0.47338107 -0.47338107 -0.47338107  2.01186954]]
```

E) The A in $A = PD^{1/2}$ is from the spectral/eigen decomposition of Σ. It is another variation on the square root of Σ. In this example, A is:

In [8]:
```
spectral_components = LA.eigh(Sigma)
```

In [9]:
```
p = spectral_components[1]
dsqrt = np.diag(np.sqrt(spectral_components[0]))
(p @ dsqrt).round(8)
```

Out[9]:
```
array([[-0.39303622,  0.        ,  0.        , -0.07431374,  0.91651514],
       [ 0.02630509,  0.        ,  0.        ,  0.39913412,  0.91651514],
       [ 0.12224371, -0.0806617 , -0.35612782, -0.10827346,  0.91651514],
       [ 0.12224371,  0.34874659,  0.10820883, -0.10827346,  0.91651514],
       [ 0.12224371, -0.26808489,  0.24791899, -0.10827346,  0.91651514]])
```

In [10]:
```
# We can reconstruct the original as desired
p @ dsqrt @ dsqrt @ p.T
```

Out[10]:
```
array([[1. , 0.8, 0.8, 0.8, 0.8],
       [0.8, 1. , 0.8, 0.8, 0.8],
       [0.8, 0.8, 1. , 0.8, 0.8],
       [0.8, 0.8, 0.8, 1. , 0.8],
       [0.8, 0.8, 0.8, 0.8, 1. ]])
```

F) Simulate 10,000 observations iid, $N(0, \Sigma)$ and calculate the MLE of μ and Σ. The MLE of μ is a vector of $\bar X_i$. The MLE of Σ is $\frac{1}{n}\sum(X_i - \bar X)(X_i - \bar X)'$. It is a baised estimator.

We sample this data by drawing from the standard normal and calculating $Y = \mu + PD^{1/2}Z$

In [11]:
```
# Draw from the standard normal and scale
simdata = p @ dsqrt @ np.random.normal(size=(5, 10000))
df = pd.DataFrame(simdata).T
df.head(10)
```

Out[11]:

	0	1	2	3	4
0	0.194507	-0.606890	0.176470	-1.087759	-0.515141
1	0.578737	0.199670	0.395919	-0.014343	-0.625791
2	-0.221497	0.253363	-0.109596	0.526614	-0.295863
3	0.784337	0.742107	1.075592	1.454302	1.372609
4	-0.751715	-0.450782	-0.803568	-1.472787	-1.057527
5	-1.876924	-1.327432	-0.355233	-1.907918	-0.744109
6	1.127785	-0.231445	0.351097	0.470698	0.336787
7	-0.114207	0.731383	0.679120	0.441572	1.214680
8	0.013644	0.410002	0.770535	0.155117	0.302383
9	-0.221710	-0.280177	-0.119045	0.088447	-0.801672

In [12]:
```
# Calculate Xbar in pandas
xbar = df.apply(np.mean, axis=0).values
display(Math(r'\hat\mu :'))
print(xbar)
```

$\displaystyle \hat\mu :$

```
[0.01237842 0.00842801 0.00486766 0.00474506 0.00719187]
```

In [13]:
```
# Loop-de-loop
sighat = np.zeros(Sigma.shape)
for idx, row in df.iterrows():
    tmp = (row.values-xbar)[:, np.newaxis]
    sighat += tmp @ tmp.T
sighat /= df.shape[0]
display(Math(r'\hat\Sigma :'))
print(sighat)
```

$\displaystyle \hat\Sigma :$

```
[[1.03051122 0.83320672 0.829584   0.83699397 0.83297075]
 [0.83320672 1.02913912 0.82751446 0.83423774 0.83246174]
 [0.829584   0.82751446 1.0255583  0.83542976 0.82872725]
 [0.83699397 0.83423774 0.83542976 1.04666139 0.84102752]
 [0.83297075 0.83246174 0.82872725 0.84102752 1.04253793]]
```

G) Repeat the above with $n=50$

In [14]:

```
# Draw from the standard normal and scale
simdata1 = p @ dsqrt @ np.random.normal(size=(5, 50))
df1 = pd.DataFrame(simdata1).T
df1.head(10)
# Calculate Xbar in pandas
xbar1 = df1.apply(np.mean, axis=0).values
display(Math(r'\hat\mu :'))
print(xbar1)
# Loop-de-loop
sighat1 = np.zeros(Sigma.shape)
for idx, row in df1.iterrows():
    tmp = (row.values-xbar1)[:, np.newaxis]
    sighat1 += tmp @ tmp.T
sighat1 /= df1.shape[0]
display(Math(r'\hat\Sigma :'))
print(sighat1)
```

$\displaystyle \hat\mu :$

```
[0.10685611 0.20621629 0.11259098 0.11403999 0.1126731 ]
```

$\displaystyle \hat\Sigma :$

```
[[0.84077475 0.73495219 0.53862276 0.74153233 0.66754285]
 [0.73495219 0.80476525 0.54879704 0.7278729  0.65249694]
 [0.53862276 0.54879704 0.65992149 0.58655239 0.53532496]
 [0.74153233 0.7278729  0.58655239 0.96225316 0.70484177]
 [0.66754285 0.65249694 0.53532496 0.70484177 0.77125384]]
```

G) The MLE of L is the Cholesky decomposition of the MLE of Σ.

Part 2: Write function to evaluate the log-likelihood of MVN.

In [15]:

```
def logL(Y, mu, Sigma):
    # Check Sigma is positive definite
    if not np.all(LA.eigvals(Sig_true) > 0):
        return np.nan
    cost = np.log(abs(LA.det(Sigma))) * Y.shape[0]
    # Use the Mahalanobis distance bulitin to vectorize
    Sinv = LA.inv(Sigma)
    for i in range(Y.shape[0]):
        cost += distance.mahalanobis(Y[i, :], mu, Sinv)**2
    # Scale cost and return
    cost *= -0.5
    return(cost)
```

Fix arbitrary values for μ, Σ and test a range of values to maximize logL

In [16]:

```
# True means
mu_true = np.array([5, -2])
# True Sigma, verify is positive definite
Sig_true = np.array([[2, .65],[.65, 1.25]])
print(np.all(LA.eigvals(Sig_true) > 0))
X = np.random.multivariate_normal(mu_true, Sig_true, 500)
```

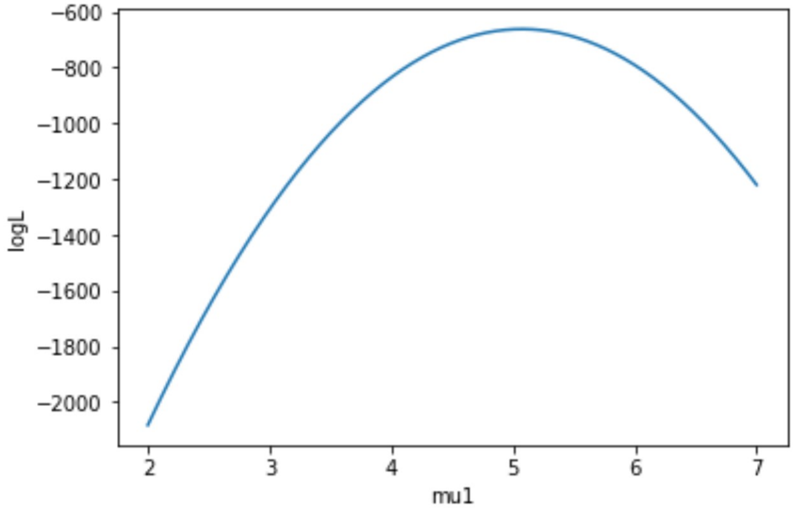
```
True
```

In [17]:

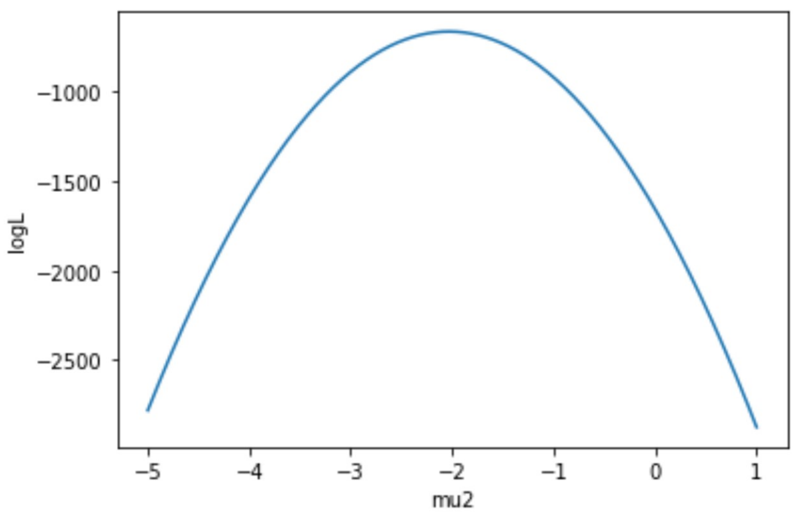
```
# Builds pd.DataFrame where all values are the true values, except
# one column will be a range of values to test
class SampleData:

    def __init__(self, target, test_n=1000, mu_true=mu_true, Sig_true=Sig_true
        self.target = target
        self.test_n = test_n
        self.mu_true = mu_true
        self.Sig_true = Sig_true
        self.build_target_data()
        self.data = self.build_test_data()

    def build_target_data(self):
        self.target_data = {
        "mu1" : np.linspace(2, 7, num=self.test_n),
        "mu2" : np.linspace(-5, 1, num=self.test_n),
        "sig11" : np.linspace(0.5, 5, num=self.test_n),
        "sig12" : np.linspace(-1, 1, num=self.test_n),
        "sig22" : np.linspace(0.5, 5, num=self.test_n)
    }

    def build_test_data(self):
        data = {
            "mu1" : np.repeat(self.mu_true[0], self.test_n),
            "mu2" : np.repeat(self.mu_true[1], self.test_n),
            "sig11" : np.repeat(self.Sig_true[0,0], self.test_n),
            "sig12" : np.repeat(self.Sig_true[0,1], self.test_n),
            "sig22" : np.repeat(self.Sig_true[1,1], self.test_n)
        }
        data[self.target] = self.get_target_values()
        return(pd.DataFrame(data))

    def get_target_values(self):
        try:
            data = self.target_data[self.target]
            return(data)
        except ValueError:
            valid = ",".join(list(self.target_data.keys()))
            print(f"Please select one of the following: {valid}")
            raise
```

In [18]:

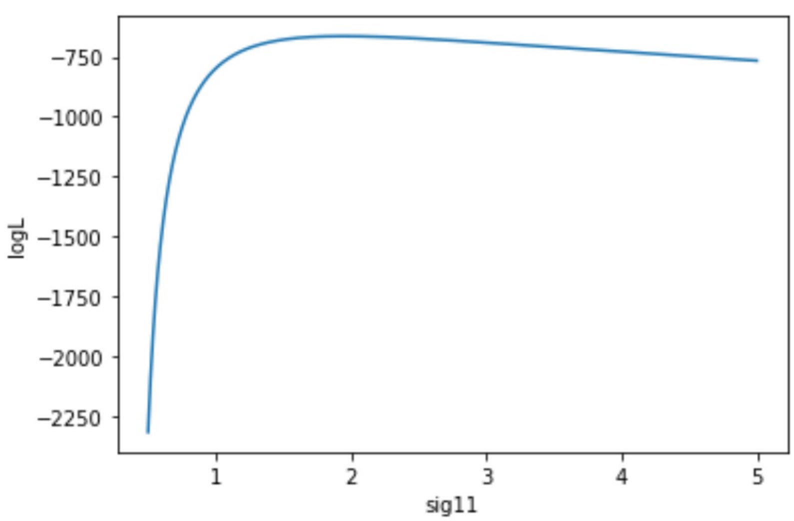
```
for item in ["mu1", "mu2", "sig11", "sig12", "sig22"]:
    tmp = SampleData(item).data
    tmp["logL"] = tmp.apply(lambda q: logL(X, q[0:2], np.array([[q[2],q[3]],
    plt.plot(tmp[item], tmp["logL"])
    plt.xlabel(item)
    plt.ylabel("logL")
    plt.show()
```



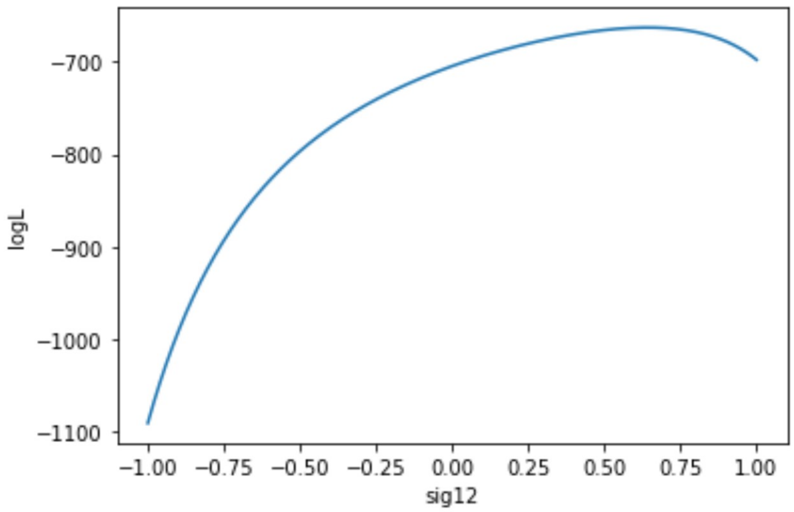
−600
−800
−1000
−1200
−1400
−1600
−1800
−2000
logL
2
3
4
5
6
7
mu1

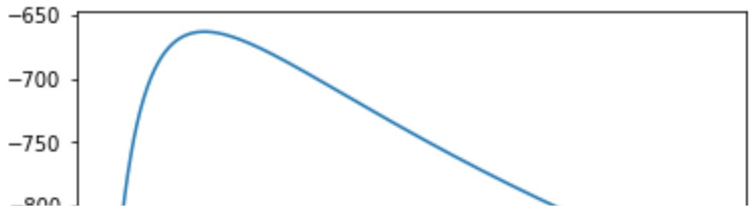


−1000
−1500
−2000
−2500
logL
−5
−4
−3
−2
−1
0
1
mu2



−750
−1000
−1250
−1500
−1750
−2000
−2250
logL
1
2
3
4
5
sig11



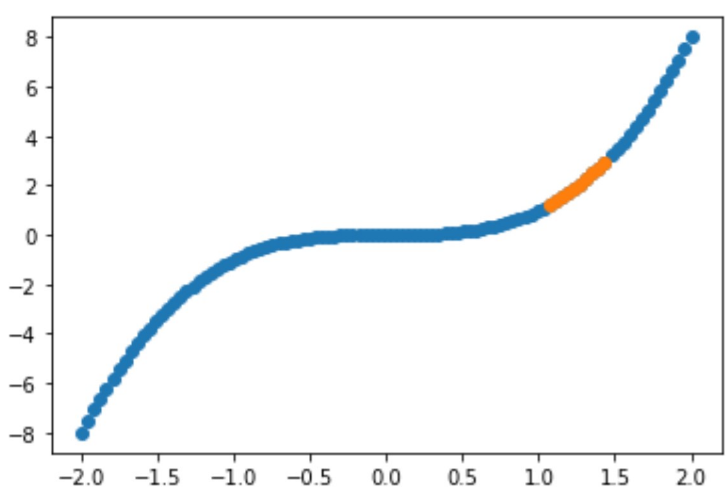


Problem 3: Gaussian Process

In [19]:
```
# Generate the entire dataset
n = 100
x = np.linspace(-2, 2, num=n)
fx = x**3
# Index the known vs uknown data
obs = list(range( 75))
obs.extend(list(range(86, 100)))
y = list(range(76,86))
print(y)
X = x[obs]
# Plot the data
plt.scatter(x, fx)
plt.scatter(x[y], fx[y])
```

```
[76, 77, 78, 79, 80, 81, 82, 83, 84, 85]
```

Out[19]: `<matplotlib.collections.PathCollection at 0x1f0b7389580>`



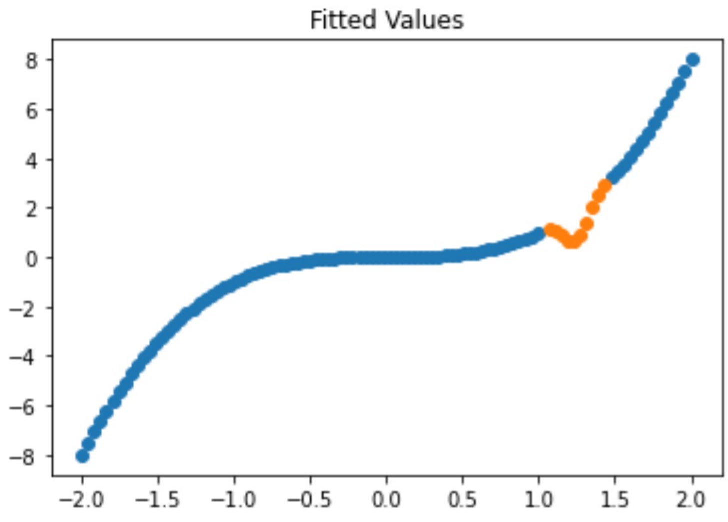
In [20]:
```
# test some values of sigf, l
l = 0.1
sigmaf = 0.1
distances = x - x[:, np.newaxis]
sigma = sigmaf**2 * np.exp(-(distances**2/l**2/2))
```

In [21]:
```
# Calculate Y | X
sig11 = sigma[obs, :][:, obs]
sig22 = sigma[y, :][:, y]
sig12 = sigma[obs, :][:, y]
sig21 = sig12.T

sig11inv = LA.inv(sig11)
sigbar = sig22 - LA.multi_dot([sig21, sig11inv, sig12])
mubar = sig21 @ sig11inv @ fx[obs]
```

In [22]:
```
# Fit yhat
yhat = np.random.multivariate_normal(mubar, sigbar)
```

In [23]:
```
plt.scatter(x[obs], fx[obs])
plt.scatter(x[y], yhat)
plt.title("Fitted Values")
```

Out[23]:
```
Text(0.5, 1.0, 'Fitted Values')
```



The values (.1, .1) were chosen because many other nearby values resutled in correlation matrices that were not full rank. Larger values resulted in worse fits.

$Y | X$ is a good generic approximation of the true values of Y

In [ ]: