Linear Regression Hand Implementation

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About The Data

I used "Energy efficiency Data Set" from UCI Machine Learning Repository (https://archive.ics.uci.edu/ml/datasets/Energy+efficiency (https://archive.ics.uci.edu/ml/datasets/Energy+efficiency))

Explanation about the data is,

Data Set Information:

"We perform energy analysis using 12 different building shapes simulated in Ecotect. The buildings differ with respect to the glazing area, the glazing area distribution, and the orientation, amongst other parameters. We simulate various settings as functions of the afore-mentioned characteristics to obtain 768 building shapes. The dataset comprises 768 samples and 8 features, aiming to predict two real valued responses. It can also be used as a multi-class classification problem if the response is rounded to the nearest integer."

and, this data's feature values (or variable, attributes) is like that

Attribute Information:

"The dataset contains eight attributes (or features, denoted by X1...X8) and two responses (or outcomes, denoted by y1 and y2). The aim is to use the eight features to predict each of the two responses. "

"Specifically: X1 Relative Compactness X2 Surface Area X3 Wall Area X4 Roof Area X5 Overall Height X6 Orientation X7 Glazing Area X8 Glazing Area Distribution y1 Heating Load y2 Cooling Load"

Purpose of The Report

I used X1~X8 as observation value, and predict y1 and y2 from them by linear regression.

this data set have 768 samples. I use 80% of them for fitting, 20% of them varidation and test.

At first, I get the data as DataFrame object using pandas, and I will show how the data is like.

In [1]:

```
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
import numpy as np
import warnings
warnings.simplefilter(action='ignore', category=FutureWarning)
```

In [2]:

```
import pandas as pd
book = pd.ExcelFile("/Users/daigofujiwara/Documents/授業資料/パターン認識特論/ENB2012_data.xlsx")
df = book.parse("Sheet1", header=0)
df.head()
```

Out[2]:

	X1	X2	X3	X4	X5	X6	X7	X8	Y1	Y2
0	0.98	514.5	294.0	110.25	7.0	2	0.0	0	15.55	21.33
1	0.98	514.5	294.0	110.25	7.0	3	0.0	0	15.55	21.33
2	0.98	514.5	294.0	110.25	7.0	4	0.0	0	15.55	21.33
3	0.98	514.5	294.0	110.25	7.0	5	0.0	0	15.55	21.33
4	0.90	563.5	318.5	122.50	7.0	2	0.0	0	20.84	28.28

The data is just like this. Next I explain about Linear Regression with math and show the code.

About Linear Regression

Using an input (feature) D-dimenssional vector sample

$$\boldsymbol{x}_i = (x_1, x_2, \ldots, x_D)^{\mathrm{T}} (i = 1, \ldots, N)$$

General regression model is writen in,

$$y(x, w) = \sum_{j=0}^{M-1} w_j \phi_j(x) = \boldsymbol{w}^{\top} \boldsymbol{\phi}(\boldsymbol{x})$$

where,

$$\boldsymbol{w} = (w_0, \ldots, w_{M-1})^{\top}, \boldsymbol{\phi} = (\phi_0, .., \phi_{M-1})^{\mathrm{T}}, \text{ and } \phi_0(\boldsymbol{x}) = 1$$

now, I use m dimessional polynomial basis function, so $\boldsymbol{\phi}(\boldsymbol{x})$ is that

$$\boldsymbol{\phi} = \left(1, x_1, x_1^2, \ldots, x_1^m, x_2, \ldots, x_2^m, x_3, \ldots, x_D^m\right)^{\top}$$

then, $M = D * m + 1$

We want to select the model which minimizes Sum of Squared Error (SSE):

$$E_D(\boldsymbol{w}) = \frac{1}{2} \sum_{n=1}^{N} \left\{t_n - \boldsymbol{w}^{\top} \boldsymbol{\phi}\left(\boldsymbol{x}_n\right)\right\}^2$$

the $\boldsymbol{w}_{ML}$ which minimize E_D can be solved analytically, like this.

$$\begin{aligned}
w_{\mathrm{ML}} &= \arg\min_{w} \frac{1}{2} \sum_{n=1}^{N} \left\{t_n - \boldsymbol{w}^{\top} \boldsymbol{\phi}\left(\boldsymbol{x}_n\right)\right\}^2 \\
0 &= \nabla_{\boldsymbol{w}} E_D(\boldsymbol{w}) \\
&= \sum_{n=1}^{N} \left\{t_n - \boldsymbol{w}^{\top} \boldsymbol{\phi}\left(\boldsymbol{x}_n\right)\right\} \boldsymbol{\phi}\left(\boldsymbol{x}_n\right)^{\top} \\
\boldsymbol{w}_{\mathrm{ML}} &= \left(\boldsymbol{\Phi}^{\top} \boldsymbol{\Phi}\right)^{-1} \boldsymbol{\Phi}^{\top} \mathbf{t} = \boldsymbol{\Phi}^{\dagger} \mathbf{t}
\end{aligned}$$

So it can be numerically calculated, this is the code which calculates w_{ML} and make polynomial basis function.

In [3]:

```
class PolynomialBasisFunction:

    def __init__(self,m):
        self.m =  m#べき級数の次元

    def getphi(self,x):
        self.phi=np.ones(self.m*x.shape[0]+1)
        for i in range(x.shape[0]):
            for j in range (self.m):
                self.phi[i*self.m+j+1]= np.power(x[i], j+1)

        return self.phi

    def getm(self):
        return self.m
```

In [4]:

```
ass LinearRegression:

 def __init__(self, basisFunction):
    self.basis = basisFunction
    self.w = "NULL"

 def fittingW(self, X, y):#引数は学習用データ
    #計画行列の初期化
    designMatrix = np.zeros((X.shape[0], X.shape[1]*self.basis.getm()+1))#X.shape=N:データ数, self.X.sha

    for i in range (X.shape[0]):
       designMatrix[i] = self.basis.getphi(X[i])

    TransM = designMatrix.T
    MultiM=np.dot(TransM,designMatrix)
    InvM=np.linalg.inv(MultiM)

    psd_inv = np.dot(InvM, TransM)#擬似逆行列

    self.w = np.dot(psd_inv,y)
    return self.w

 def predictY(self, X):#引数はテスト用データ
    #計画行列の初期化
    designMatrix = np.zeros((X.shape[0], X.shape[1]*self.basis.getm()+1))#X.shape=N:データ数, self.X.sha

    for i in range(X.shape[0]):
       designMatrix[i] = self.basis.getphi(X[i])

    if self.w == "NULL":
       print("haven't optimized !!")

    else:
       y=np.dot(designMatrix, self.w)
       return y
```

Analysis and Experiment

Using these classess, I tried regression according to dimenssion parameter $m = 1$, and $m = 2$. After that I will compare them.

Analysis and Experiment(m=1)

In [5]:

```
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split
```

In [6]:

```
#dataのnp.arrayとしての取り出し
X = df[["X1", "X2", "X3", "X4", "X5", "X6", "X7", "X8"]].values
Y = df[["Y1","Y2"]].values

# 標準化
sc_x = StandardScaler()
sc_y = StandardScaler()
X_std = sc_x.fit_transform(X)
Y_std = sc_y.fit_transform(Y)
```

In [7]:

```


# 学習用データとテスト用データに分割
X_train, X_test, Y_train, Y_test = train_test_split(X_std, Y_std, test_size=0.2, random_state=0)

#basisFunction
basisFunction=PolynomialBasisFunction(1)

# regression model
regressionModel = LinearRegression(basisFunction)
regressionModel.fittingW(X_train, Y_train)
```

Out[7]:

```
array([[-5.42855754e-03,  1.03261296e-03],
       [-1.09129452e+00, -1.19242699e+00],
       [-1.96446300e+00, -2.21293803e+00],
       [ 7.44193409e-01,  7.89699221e-01],
       [ 9.43914197e-01,  1.18071216e+00],
       [ 7.03358957e-01,  7.94908129e-01],
       [-2.31683218e-03,  1.68597622e-02],
       [ 2.61549551e-01,  2.10993165e-01],
       [ 2.45409712e-02,  3.87468965e-03]])
```

this is the optimaized weight w_{ML}. The left colm is for $y1$, and the other is for $y2$.

In [8]:

```
# predicting
Y_train_pred = regressionModel.predictY(X_train)
Y_test_pred = regressionModel.predictY(X_test)

#標準化を戻す
temp=sc_y
Y_train = sc_y.inverse_transform(Y_train)
sc_y=temp
Y_test = sc_y.inverse_transform(Y_test)
sc_y=temp
Y_train_pred = sc_y.inverse_transform(Y_train_pred)
sc_y=temp
Y_test_pred = sc_y.inverse_transform(Y_test_pred)


y1_train=(Y_train.T[0]).T
y2_train=(Y_train.T[1]).T
y1_test=(Y_test.T[0]).T
y2_test=(Y_test.T[1]).T
y1_train_pred=(Y_train_pred.T[0]).T
y2_train_pred=(Y_train_pred.T[1]).T
y1_test_pred=(Y_test_pred.T[0]).T
y2_test_pred=(Y_test_pred.T[1]).T
```

Evaluation

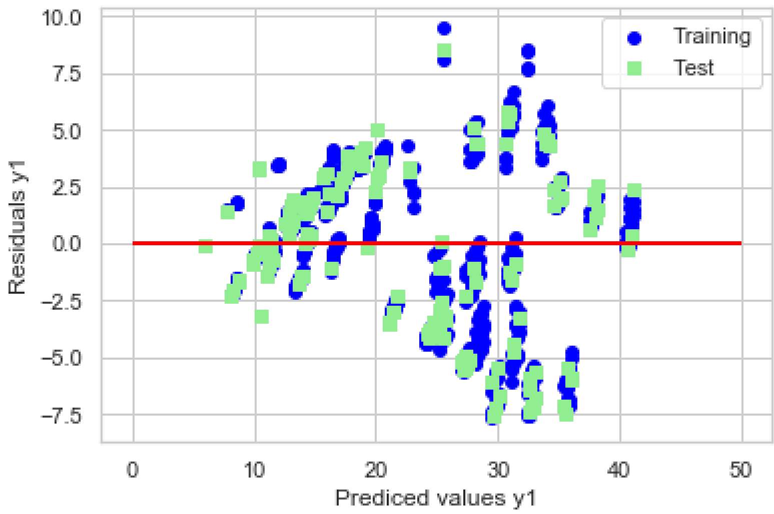
I taked visual evaluation to the accuracy of prediction and quantitative analysis . I will show the plot. As a quantittative analysis, I used Mean Squared Error (MSE).

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y^{(i)} - \hat{y^{(i)}})$$

y1

In [9]:

```
sns.set(style="whitegrid", context="notebook")
plt.scatter(y1_train_pred, y1_train_pred - y1_train,
        c="blue", marker="o", label="Training")
plt.scatter(y1_test_pred, y1_test_pred - y1_test,
        c="lightgreen", marker="s", label="Test")
plt.xlabel("Prediced values y1")
plt.ylabel("Residuals y1")
plt.legend()
plt.hlines(y=0, xmin=0, xmax=50, lw=2, color="red")
plt.show()
```



In [10]:

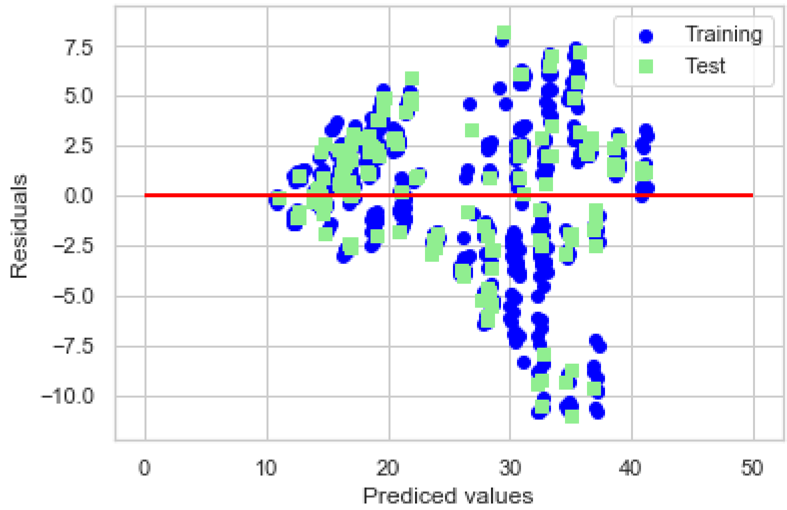
```
from sklearn.metrics import mean_squared_error as mse

print("MSE train: %.3f, test: %.3f" % (mse(y1_train, y1_train_pred), mse(y1_test, y1_test_pred)))
```

MSE train: 10.724, test: 12.517

y2

In [11]:

```
sns.set(style="whitegrid", context="notebook")
plt.scatter(y2_train_pred, y2_train_pred - y2_train,
        c="blue", marker="o", label="Training")
plt.scatter(y2_test_pred, y2_test_pred - y2_test,
        c="lightgreen", marker="s", label="Test")
plt.xlabel("Prediced values")
plt.ylabel("Residuals")
plt.legend()
plt.hlines(y=0, xmin=0,xmax=50, lw=2, color="red")
plt.show()
```



In [12]:

```
from sklearn.metrics import mean_squared_error as mse

print("MSE train: %.3f, test: %.3f" % (mse(y2_train, y2_train_pred), mse(y2_test, y2_test_pred)))
```

MSE train: 12.389, test: 13.452

Analysis and Expwriment(m=2)

Next,I try basis function's parameter m=2.

In [13]:

```
#dataのnp.arrayとしての取り出し
X = df[["X1", "X2", "X3", "X4", "X5", "X6", "X7", "X8"]].values
Y = df[["Y1","Y2"]].values

# 標準化
sc_x = StandardScaler()
sc_y = StandardScaler()
X_std = sc_x.fit_transform(X)
Y_std = sc_y.fit_transform(Y)

# 学習用データとテスト用データに分割
X_train, X_test, Y_train, Y_test = train_test_split(X_std, Y_std, test_size=0.2, random_state=0)

#basisFunction
basisFunction=PolynomialBasisFunction(2)

# regression model
regressionModel = LinearRegression(basisFunction)
regressionModel.fittingW(X_train, Y_train)

# predicting
Y_train_pred = regressionModel.predictY(X_train)
Y_test_pred = regressionModel.predictY(X_test)

#標準化を戻す
temp=sc_y
Y_train = sc_y.inverse_transform(Y_train)
sc_y=temp
Y_test = sc_y.inverse_transform(Y_test)
sc_y=temp
Y_train_pred = sc_y.inverse_transform(Y_train_pred)
sc_y=temp
Y_test_pred = sc_y.inverse_transform(Y_test_pred)


y1_train=(Y_train.T[0]).T
y2_train=(Y_train.T[1]).T
y1_test=(Y_test.T[0]).T
y2_test=(Y_test.T[1]).T
y1_train_pred=(Y_train_pred.T[0]).T
y2_train_pred=(Y_train_pred.T[1]).T
y1_test_pred=(Y_test_pred.T[0]).T
y2_test_pred=(Y_test_pred.T[1]).T
```

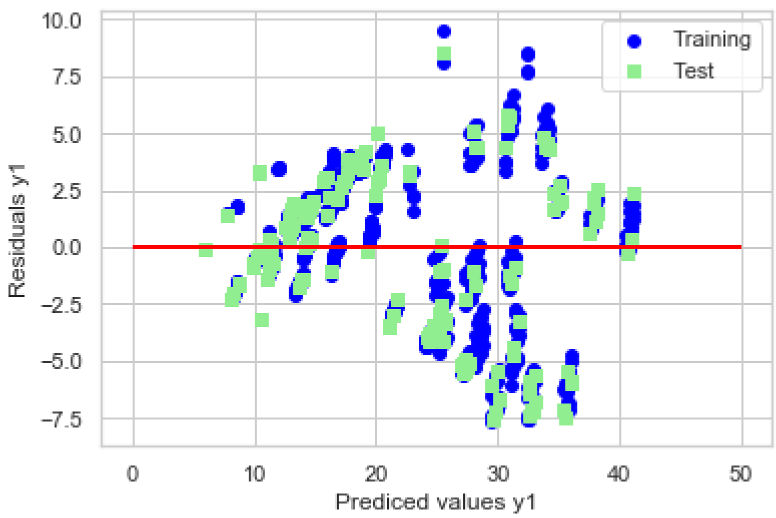
```
---------------------------------------------------------------------------
LinAlgError                               Traceback (most recent call last)
<ipython-input-13-a75d7102b2da> in <module>
     17 # regression model
     18 regressionModel = LinearRegression(basisFunction)
---> 19 regressionModel.fittingW(X_train, Y_train)
     20 
     21 # predicting

<ipython-input-4-ad88af453406> in fittingW(self, X, y)
     14         TransM = designMatrix.T
     15         MultiM=np.dot(TransM,designMatrix)
---> 16         InvM=np.linalg.inv(MultiM)
     17 
     18         psd_inv = np.dot(InvM, TransM)#擬似逆行列
```

```
~/anaconda3/lib/python3.7/site-packages/numpy/linalg/linalg.py in inv(a)
    549     signature = 'D->D' if isComplexType(t) else 'd->d'
    550     extobj = get_linalg_error_extobj(_raise_linalgerror_singular)
--> 551     ainv = _umath_linalg.inv(a, signature=signature, extobj=extobj)
    552     return wrap(ainv.astype(result_t, copy=False))
    553

~/anaconda3/lib/python3.7/site-packages/numpy/linalg/linalg.py in _raise_linalgerror_
singular(err, flag)
     95
     96 def _raise_linalgerror_singular(err, flag):
---> 97     raise LinAlgError("Singular matrix")
     98
     99 def _raise_linalgerror_nonposdef(err, flag):

LinAlgError: Singular matrix
```

y1

In [14]:

```
sns.set(style="whitegrid", context="notebook")
plt.scatter(y1_train_pred, y1_train_pred - y1_train,
        c="blue", marker="o", label="Training")
plt.scatter(y1_test_pred, y1_test_pred - y1_test,
        c="lightgreen", marker="s", label="Test")
plt.xlabel("Prediced values y1")
plt.ylabel("Residuals y1")
plt.legend()
plt.hlines(y=0, xmin=0, xmax=50, lw=2, color="red")
plt.show()
```



In [15]:

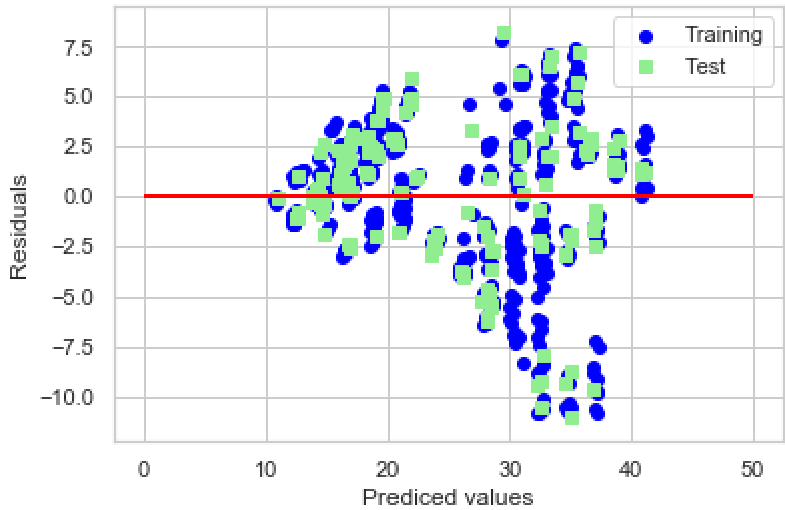
```
from sklearn.metrics import mean_squared_error as mse

print("MSE train: %.3f, test: %.3f" % (mse(y1_train, y1_train_pred), mse(y1_test, y1_test_pred)))
```

MSE train: 10.724, test: 12.517

y2

In [16]:

```
sns.set(style="whitegrid", context="notebook")
plt.scatter(y2_train_pred, y2_train_pred - y2_train,
        c="blue", marker="o", label="Training")
plt.scatter(y2_test_pred, y2_test_pred - y2_test,
        c="lightgreen", marker="s", label="Test")
plt.xlabel("Prediced values")
plt.ylabel("Residuals")
plt.legend()
plt.hlines(y=0, xmin=0,xmax=50, lw=2, color="red")
plt.show()
```



In [17]:

```
from sklearn.metrics import mean_squared_error as mse

print("MSE train: %.3f, test: %.3f" % (mse(y2_train, y2_train_pred), mse(y2_test, y2_test_pred)))
```

MSE train: 12.389, test: 13.452

coment

According to MSE data below, clearly m=1 model is better than m=2 one. It may be caused by overfitting, because the number of data is relatively few, and as m get bigger, the complexity of this model (the dimenssion of basis function : M) increase drasticaly.

m=1
MSE train: 8.415, test: 10.822

m=2
MSE train: 141073366089532411215872.000, test: 156393509577783081172992.000

Additional Research : Gaussian Basis Function

I try to change basis function polynominal to Gaussian. Newly we define GaussianBasisFunction class. This research is for only y1. Now, I use m dimessional Gaussian basis function, so $\phi(x)$ is that

$$\boldsymbol{\phi} = \left(1, \phi_{1,1}, \phi_{1,2}, \ldots, \phi_{1,m}, \phi_{2,1}, \ldots, \phi_{2,m}, \phi_{3,1}, \ldots, x_{D,m}\right)^\top$$

where

$$\phi_{i,j} = \exp\left[-\frac{\left(x_i - \mu_j\right)^2}{2s^2}\right]$$

In [18]:

```
class GaussianBasisFunction:
    def __init__(self,m):
        self.s2=1
        self.m=m

    def getphi(self,x):
        mu=np.arange(self.m)
        mu=mu/self.m
        self.phi=np.ones(self.m*x.shape[0]+1)
        for i in range(x.shape[0]):
            for j in range (self.m):
                self.phi[i*self.m+j+1]= np.exp(-(x[i]-mu[j])*(x[i]-mu[j])/(2*self.s2))

        return self.phi

    def getm(self):
        return self.m
```

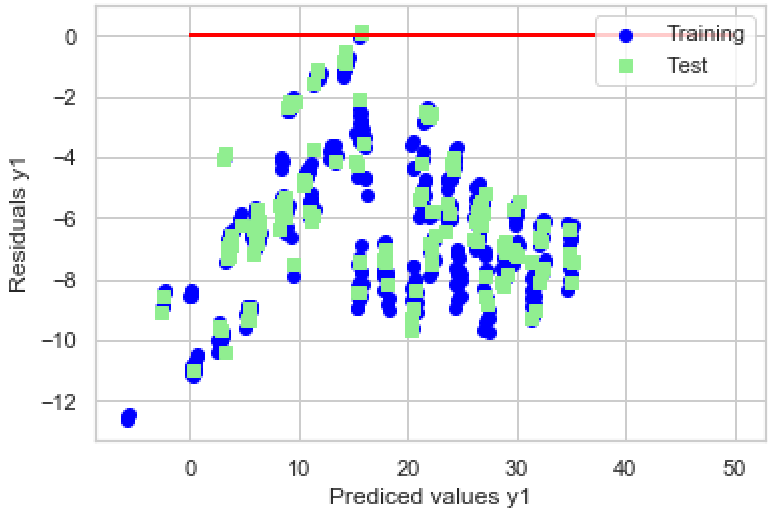
m=3, y1

In [19]:

```
#dataのnp.arrayとしての取り出し
X = df[["X1", "X2", "X3", "X4", "X5", "X6", "X7", "X8"]].values
Y = df[["Y1","Y2"]].values

# 標準化
sc_x = StandardScaler()
sc_y = StandardScaler()
X_std = sc_x.fit_transform(X)
Y_std = sc_y.fit_transform(Y)

# 学習用データとテスト用データに分割
X_train, X_test, Y_train, Y_test = train_test_split(X_std, Y_std, test_size=0.2, random_state=0)

#basisFunction
basisFunction=GaussianBasisFunction(3)

# regression model
regressionModel = LinearRegression(basisFunction)
regressionModel.fittingW(X_train, Y_train)

# predicting
Y_train_pred = regressionModel.predictY(X_train)
Y_test_pred = regressionModel.predictY(X_test)

#標準化を戻す
temp=sc_y
Y_train = sc_y.inverse_transform(Y_train)
sc_y=temp
Y_test = sc_y.inverse_transform(Y_test)
sc_y=temp
Y_train_pred = sc_y.inverse_transform(Y_train_pred)
sc_y=temp
Y_test_pred = sc_y.inverse_transform(Y_test_pred)


y1_train=(Y_train.T[0]).T

y1_test=(Y_test.T[0]).T

y1_train_pred=(Y_train_pred.T[0]).T

y1_test_pred=(Y_test_pred.T[0]).T
```

In [20]:

```
sns.set(style="whitegrid", context="notebook")
plt.scatter(y1_train_pred, y1_train_pred - y1_train,
        c="blue", marker="o", label="Training")
plt.scatter(y1_test_pred, y1_test_pred - y1_test,
        c="lightgreen", marker="s", label="Test")
plt.xlabel("Prediced values y1")
plt.ylabel("Residuals y1")
plt.legend()
plt.hlines(y=0, xmin=0, xmax=50, lw=2, color="red")
plt.show()
```



In [21]:

```
from sklearn.metrics import mean_squared_error as mse

print("MSE train: %.3f, test: %.3f" % (mse(y1_train, y1_train_pred), mse(y1_test, y1_test_pred)))
```

MSE train: 44.009, test: 41.348

coment

Seeing the result, regression by Gaussian basis function exceeds any polynomial regression so far.

Change of MSE for m

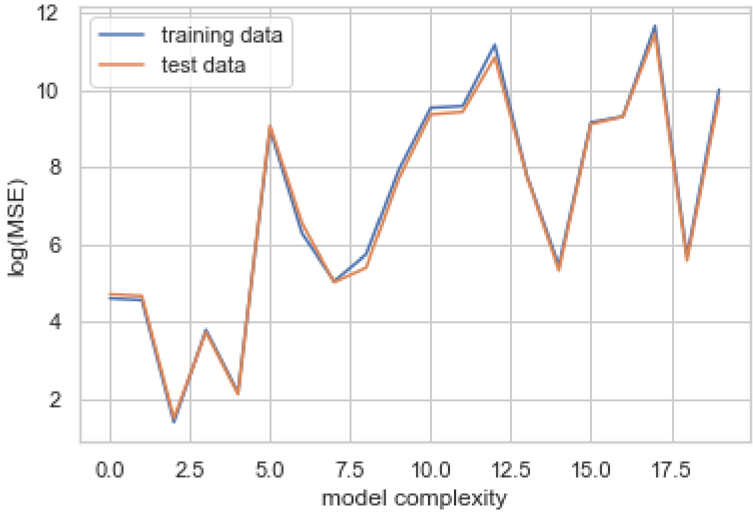
I visualize the changing of MSE as the parameter m (complexity of model) increases.

In [22]:

```
M = 20# max model complexity to search
mse_train = []
mse_test = []

for m in range(M):
    X = df[["X1", "X2", "X3", "X4", "X5", "X6", "X7", "X8"]].values
    Y = df[["Y1","Y2"]].values

    # 標準化
    sc_x = StandardScaler()
    sc_y = StandardScaler()
    X_std = sc_x.fit_transform(X)
    Y_std = sc_y.fit_transform(Y)

    # 学習用データとテスト用データに分割
    X_train, X_test, Y_train, Y_test = train_test_split(X_std, Y_std, test_size=0.2, random_state=0)

    #basisFunction
    basisFunction=GaussianBasisFunction(m)

    # regression model
    regressionModel = LinearRegression(basisFunction)
    regressionModel.fittingW(X_train, Y_train)

    # predicting
    Y_train_pred = regressionModel.predictY(X_train)
    Y_test_pred = regressionModel.predictY(X_test)

    #標準化を戻す
    temp=sc_y
    Y_train = sc_y.inverse_transform(Y_train)
    sc_y=temp
    Y_test = sc_y.inverse_transform(Y_test)
    sc_y=temp
    Y_train_pred = sc_y.inverse_transform(Y_train_pred)
    sc_y=temp
    Y_test_pred = sc_y.inverse_transform(Y_test_pred)

    y1_train=(Y_train.T[0]).T

    y1_test=(Y_test.T[0]).T

    y1_train_pred=(Y_train_pred.T[0]).T

    y1_test_pred=(Y_test_pred.T[0]).T


    # the MSE is recoded
    mse_train.append(mse(y1_train, y1_train_pred))
    mse_test.append(mse(y1_test, y1_test_pred))
```

In [23]:

```
fig = plt.figure()
ax =fig.add_subplot(111)
ax.plot(range(len(mse_train)), np.log(mse_train), label="training data")
ax.plot(range(len(mse_test)), np.log(mse_test), label="test data")
ax.set_xlabel("model complexity")
ax.set_ylabel("log(MSE)")
plt.legend()
plt.show()
```



Conclusion

This graph and these researches shows that complexity sometimes make regression model worse, and a model have the best degree of complexity for its own. It can be also said that, in linear regression model, according to the data treationg, its accuracy depends so much on basis function.