# Results

December 12, 2018

# 1 Results of feature importance evaluations

# 1.1 Imports

```
In [1]: ## generals
        import pandas as pd
        import numpy as np
        import timeit
        from functools import partial
        import matplotlib.pyplot as plt
        from scipy.io import loadmat
        import matplotlib.pyplot as plt
        import time
        ## hoggorm
        import hoggorm as ho
        ##sklearn
        from sklearn.cross_decomposition import PLSRegression
        import sklearn.datasets
        from sklearn.exceptions import NotFittedError
        from sklearn.linear_model import Ridge
        from sklearn.model_selection import train_test_split
        from sklearn.metrics import mean_absolute_error
        ## mlxtend
        from mlxtend.feature_selection import ExhaustiveFeatureSelector as EFS
        ##selfmade
        from VIP import VIP
        from sMCf import sMC
        from IPW import IPW
```

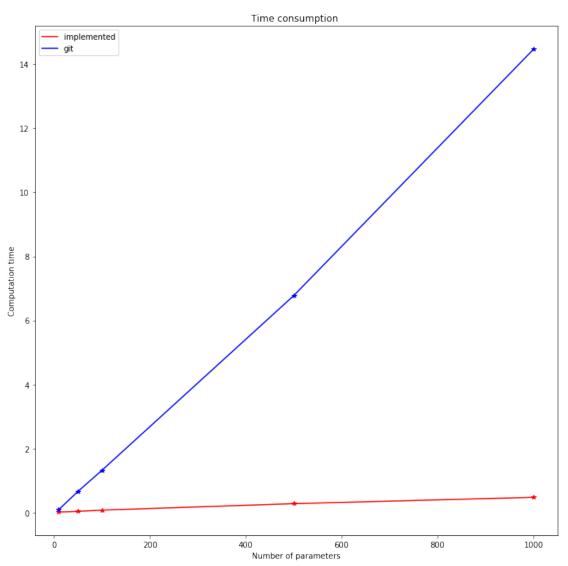
#### 1.2 VIP

# 1.2.1 intuitive vrs implemented

```
In [2]: def VIP_implemented(pls,opt=None,p=None):
            Computes the importances to the data given
            Get a quantified importance value for each parameter in the matrix X
            a set of column vectors equal in length to the number of variables
            included in the model. It contains one column of VIP scores for each
            predicted y-block column.
            Parameters
            _____
            pls : object
                object from PLS regression with atributes y_loadings_, x_scores_
                and x_weights_.
            opt : int
                optimal number of components of PLS model.
            p:int
                number of variables in PLS model.
            Returns
            _____
            :returns value: a nx1 vector, where n are the number of features in x
            :type value: vector
            11 11 11
           pls = pls
           p = len(pls.coef_) if p is None else p
            opt = None if opt is None else opt
           q = pls.y_loadings_
            t = pls.x_scores_
            W = pls.x_weights_
            WW = np.divide(W*W , np.ones((p,1))*sum(W*W)) # evt np.sum(W*W,axis=0)
            Q2TT = (np.dot(np.dot((q*q)[0:opt],t[:,0:opt].T),t[:,0:opt]))
            importances = np.sqrt(p*np.sum(np.ones((p,1))*Q2TT*WW[:,:opt],axis=1)/np.sum(Q2TT)
            return importances
        def vip_git(model):
```

```
11 11 11
            Aquired from https://github.com/scikit-learn/scikit-learn/issues/7050
            t = model.x_scores_
            w = model.x_weights_
            q = model.y_loadings_
           p, h = w.shape
            vips = np.zeros((p,))
            s = np.diag(t.T @ t @ q.T @ q).reshape(h, -1)
            total_s = np.sum(s)
            for i in range(p):
                \#weight = np.array([(w[i,j] / np.linalg.norm(w[:,j]))**2 for j in range(h)])
                \#weight = np.array([(w[i,j] / np.linalg.norm(w[:,j]))**2 for j in range(h)])
                \#weight = np.divide(w[i,:],np.linalg.norm(w))**2
                \#inni = 2*s.T @np.divide(w[i,:],np.linalg.norm(w))**2
                #vips[i] = np.sqrt(p*(inni)/total_s)
                weight = np.array([ (w[i,j] / np.linalg.norm(w[:,j]))**2 for j in range(h) ])
                vips[i] = np.sqrt(p*(s.T @ weight)/total_s)
                #vips[i] = np.sqrt(p*(s.T @ weight)/total_s)
            return vips
In [3]: data = sklearn.datasets.load_boston()
       X = data['data']
        y = data['target']
       pls = PLSRegression()
       pls.fit(X,y)
       vip1 = VIP_implemented(pls)
        vip2 = vip_git(pls)
1.2.2 VIP scores
In [4]: np.round(vip1,14) == np.round(vip2,14)
Out[4]: array([ True, True, True, True, True, True, True, True, True,
                True, True,
                              True, True])
1.2.3 Speed
In [5]: times1 = timeit.Timer(partial(VIP_implemented, pls)).repeat(3, 1000)
        times2 = timeit.Timer(partial(vip_git, pls)).repeat(3, 1000)
        times1[0] /times2[0]
In [ ]: time_imp = []
        time_git = []
        params = [10,50,100,500,1000]#,1000,10000]#,100000]
        samples = 506
        for no_params in params:
            X_test = np.random.rand(samples,no_params)
           pls.fit(X_test,y)
```

```
time_imp.append(timeit.Timer(partial(VIP_implemented, pls)).repeat(3, 500)[0])
time_git.append(timeit.Timer(partial(vip_git, pls)).repeat(3, 500)[0])
```



# 1.3 score on Boston Housing Dataset

#### 1.3.1 VIP

```
In [9]: ##Sklearn
        Importance_Boston_VIP = pd.DataFrame(index =data['feature_names'])
        vip = VIP()
        pls_sklearn = PLSRegression(scale=False)
       pls_sklearn.fit(X,y)
        vip.fit(pls_sklearn)
        Importance_Boston_VIP['sklearn pls'] = vip.importances
        #Values from Matlab
        #Stored values from the VIP process in matlab as vipscores1.mat in the validering fold
        Importance_Boston_VIP['Matlab VIP'] = loadmat('./validering/vipscores1.mat')['values']
        # values in python from matlab PLS atributes
        #Stored values of X scores as xs.mat and weigts as w.mat from matlab pls method in the
        pls.y_loadings_ = np.array([[101.729463326136,34.0591751857485]]) # extracted y_loading
        pls.x_scores_ = loadmat('./validering/xs.mat')['Xs']
        pls.x_weights_ = loadmat('./validering/W.mat')['W']
        Importance_Boston_VIP['matlab pls'] = vip.importances
        #hoggorm PLS
        pls ho = ho.nipalsPLS1(X, y.reshape(506,1), cvType=['loo'], numComp=2)
        Importance_Boston_VIP['hoggorm pls'] = vip.importances
        # extracted from r
        Importance_Boston_VIP['R-VIP nipals pls'] = pd.Series([0.171312472, 0.709292976, 0.1774
                                                                 0.002431485, 0.056888702, 0.6
                                                                 0.152825608, 3.160193230, 0.09
                                                                 0.496683595] ,index=data['fea
        Importance_Boston_VIP
100
100
Out [9]:
                 sklearn pls Matlab VIP matlab pls hoggorm pls R-VIP nipals pls
                    0.171312
                                0.173715
                                            0.173715
                                                         0.171312
                                                                           0.171312
        CRIM
        ZN
                    0.709293
                                0.716212
                                            0.716212
                                                         0.709293
                                                                           0.709293
```

```
INDUS
            0.177492
                        0.179978
                                    0.179978
                                                  0.177492
                                                                    0.177492
CHAS
            0.005766
                        0.005796
                                    0.005796
                                                  0.005766
                                                                    0.005766
NOX
            0.002431
                        0.002465
                                    0.002465
                                                  0.002431
                                                                    0.002431
RM
            0.056889
                        0.057243
                                    0.057243
                                                  0.056889
                                                                    0.056889
AGE
            0.618079
                        0.626494
                                    0.626494
                                                  0.618079
                                                                    0.618079
DIS
            0.021929
                        0.021727
                                    0.021727
                                                  0.021929
                                                                    0.021929
RAD
            0.152826
                        0.150566
                                    0.150566
                                                                    0.152826
                                                  0.152826
TAX
            3.160193
                        3.149395
                                    3.149395
                                                  3.160193
                                                                    3.160193
PTRATIO
            0.095656
                        0.096555
                                    0.096555
                                                  0.095656
                                                                    0.095656
            1.335759
                        1.351521
                                    1.351521
                                                  1.335759
                                                                    1.335759
LSTAT
            0.496684
                        0.500895
                                    0.500895
                                                                    0.496684
                                                  0.496684
```

#### 1.3.2 sMC

```
In [10]: # sklearn
         Importance_Boston_sMC = pd.DataFrame(index = data['feature_names'])
         pls = PLSRegression(scale=False)
         pls.fit(X,y)
         smc = sMC()
         smc.fit(pls,X)
         Importance_Boston_sMC['sklearn pls'] = smc.importances
         # values from matlab
         #Stored values from the sMC process in matlab as values_smc_1.mat in the validering f
         Importance Boston_sMC['Matlab sMC'] = loadmat('./validering/values_smc 1_centered.mat
         # values in python from matlab coefficients
         # beta values from matlab are stored as beta 1 in the validering folder
         pls = PLSRegression()
         pls.fit(X,y)
         coef = loadmat('./validering/beta_1_centered.mat')['BETA']
         pls.coef_ = coef[1:] # remove interception
         smc = sMC()
         smc.fit(pls,X)
         Importance_Boston_sMC['Matlab coef'] = smc.importances
         # hoggorm pls
         #from sMCf import sMC
         pls = ho.nipalsPLS1(X, y.reshape(506,1), cvType=['loo'], numComp=2)
         smc.fit(pls,X)
         Importance_Boston_sMC['hoggorm pls'] =smc.importances
         # Values from R
         # extracted from r
         Importance_Boston_sMC['R sMC w/nipals pls'] = pd.Series([7.209326e+02, 6.146978e+02,
                                                                   3.883885e+02, 9.805696e+02,
                                                                  7.607644e+02, 2.350280e-03,
```

5.910422e+01, 6.033948e+02,

### Importance\_Boston\_sMC

100 100

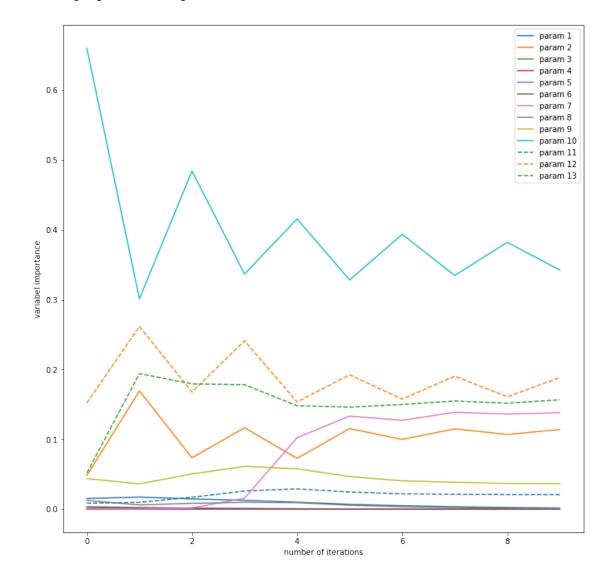
```
Out [10]:
                  sklearn pls
                                 Matlab sMC Matlab coef hoggorm pls
                   720.932559
                                                             720.932559
         CRIM
                                 720.932559
                                               720.932559
         ZN
                    614.697833
                                 614.697833
                                               614.697833
                                                             614.697833
         INDUS
                   1001.570191
                               1001.570191
                                              1001.570191
                                                            1001.570191
         CHAS
                    388.388473
                                 388.388473
                                               388.388473
                                                             388.388473
         NOX
                    980.569572
                                 980.569572
                                               980.569572
                                                             980.569572
         RM
                    542.168964
                                 542.168964
                                               542.168964
                                                             542.168964
         AGE
                   760.764384
                                 760.764384
                                               760.764384
                                                             760.764384
                                   0.002350
                                                               0.002350
         DIS
                      0.002350
                                                 0.002350
         RAD
                    27.029754
                                  27.029754
                                                27.029754
                                                              27.029754
         TAX
                    59.104216
                                  59.104216
                                                59.104216
                                                              59.104216
         PTRATIO
                    603.394756
                                 603.394756
                                               603.394756
                                                             603.394756
                   757.993942
                                 757.993942
                                               757.993942
                                                             757.993942
         В
         LSTAT
                    627.098220
                                 627.098220
                                               627.098220
                                                             627.098220
                  R sMC w/nipals pls
         CRIM
                            720.93260
         ZN
                            614.69780
         INDUS
                           1001.57000
         CHAS
                            388.38850
         NOX
                            980.56960
         RM
                            542.16900
         AGE
                            760.76440
         DIS
                              0.00235
         RAD
                             27.02975
         TAX
                             59.10422
         PTRATIO
                            603.39480
         В
                            757.99390
         LSTAT
                            627.09820
```

# 1.3.3 IPW

### sklearn

#### Out[12]: sklearn Ridge CRIM 1.799166e-03 ZN1.141085e-01 INDUS 1.665880e-10 CHAS 1.910537e-13 NOX 3.736411e-26 RM1.713835e-05 AGE 1.381398e-01 DIS 1.086916e-03 RAD 3.639848e-02 TAX 3.423726e-01 PTRATIO 2.087235e-02 1.885313e-01 LSTAT 1.566738e-01

In [13]: ipw.plot\_development()



# 1.4 Comparison

The comparioson is done with Sklearn and Hoggorm, which as been done to indicate the diffrent result with and without scaling.

Shown Below is the results obtained with scaling wich is done with sklearn and without scaling which is done with Hoggorm.

Tables of both the rank and the measure of importance have been included for both cases

#### 1.4.1 sklearn

```
In [24]: Importance_Boston_Comp = pd.DataFrame(index =data['feature_names'])
         vip = VIP()
         smc = sMC()
         ipw = IPW()
         r = Ridge()
         pls = PLSRegression(scale=True)
         pls.fit(X,y)
         vip.fit(pls)
         Importance_Boston_Comp['VIP sklearn'] = vip.importances
         smc.fit(pls,X)
         Importance_Boston_Comp['sMC sklearn'] = smc.importances
         ipw.fit(r,X,y,threshold=0)
         Importance_Boston_Comp['IPW sklearn Ridge'] = ipw.importances
         Importance_Boston_Comp
Out [24]:
                  VIP sklearn
                                sMC sklearn IPW sklearn Ridge
         CRIM
                     0.733727 7.962739e+01
                                                   1.799166e-03
         ZN
                     0.717301 3.118435e+00
                                                   1.141085e-01
         INDUS
                     0.970405 8.159210e+01
                                                   1.665880e-10
         CHAS
                     0.570576 5.055341e+02
                                                   1.910537e-13
         иох
                     0.924612 6.285301e+02
                                                   3.736411e-26
         RM
                     1.635932 5.192550e+02
                                                   1.713835e-05
         AGE
                     0.854793 1.654036e-07
                                                   1.381398e-01
         DIS
                     1.051266 3.151353e+02
                                                   1.086916e-03
         RAD
                     0.907570 2.132675e+00
                                                   3.639848e-02
         TAX
                     0.950611 6.668559e-02
                                                   3.423726e-01
         PTRATIO
                     1.012233 6.008149e+02
                                                   2.087235e-02
         В
                     0.619090 6.739726e-01
                                                   1.885313e-01
         LSTAT
                     1.475682 8.972325e+02
                                                   1.566738e-01
In [25]: Importance_Boston_Comp_no = pd.DataFrame(index =data['feature_names'])
         Importance_Boston_Comp_no['VIP sklearn pls'] = np.argsort(np.argsort(vip.importances)
         Importance_Boston_Comp_no['sMC sklearn pls'] = np.argsort(np.argsort(smc.importances)
```

```
Importance_Boston_Comp_no['IPW sklearn Ridge'] = np.argsort(np.argsort(ipw.importance)
Importance_Boston_Comp_no
```

Out[25]:		VIP	sklearn	pls	$\mathtt{sMC}$	sklearn	pls	IPW	${\tt sklearn}$	Ridge
	CRIM			10			8			8
	ZN			11			9			5
	INDUS			5			7			11
	CHAS			13			5			12
	NOX			7			2			13
	RM			1			4			10
	AGE			9			13			4
	DIS			3			6			9
	RAD			8			10			6
	TAX			6			12			1
	PTRATIO			4			3			7
	В			12			11			2
	LSTAT			2			1			3

# 1.4.2 Hoggorm

```
In [26]: Importance_Boston_Comp = pd.DataFrame(index =data['feature_names'])
         vip = VIP()
         smc = sMC()
         ipw = IPW()
         r = Ridge()
         #pls = PLSRegression()
         \#pls.fit(X,y)
         pls = ho.nipalsPLS1(X, y.reshape(506,1), cvType=['loo'], numComp=2,Xstand=False)
         vip.fit(pls)
         Importance_Boston_Comp['VIP sklearn'] = vip.importances
         smc.fit(pls,X)
         Importance_Boston_Comp['sMC sklearn'] = smc.importances
         ipw.fit(r,X,y,threshold=0)
         Importance_Boston_Comp['IPW sklearn Ridge'] = ipw.importances
         Importance_Boston_Comp
100
100
Out [26]:
                  VIP sklearn sMC sklearn IPW sklearn Ridge
```

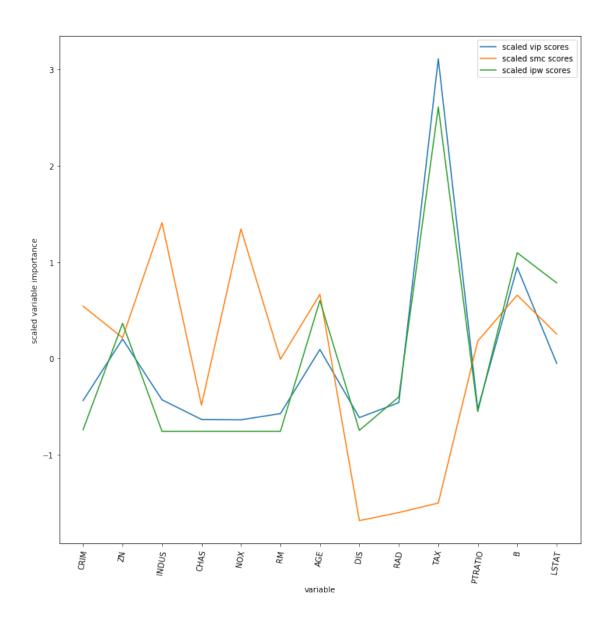
```
CRIM
           0.171312
                    720.932559
                                       1.799166e-03
ZN
                                       1.141085e-01
           0.709293 614.697833
INDUS
           0.177492 1001.570191
                                      1.665880e-10
CHAS
           0.005766 388.388473
                                       1.910537e-13
NOX
           0.002431 980.569572
                                      3.736411e-26
RM
           0.056889 542.168964
                                      1.713835e-05
```

```
AGE
            0.618079
                       760.764384
                                         1.381398e-01
DIS
            0.021929
                         0.002350
                                         1.086916e-03
R.AD
            0.152826
                        27.029754
                                         3.639848e-02
TAX
            3.160193
                       59.104216
                                         3.423726e-01
                                         2.087235e-02
PTRATIO
            0.095656
                       603.394756
            1.335759
                       757.993942
                                         1.885313e-01
LSTAT
            0.496684
                       627.098220
                                         1.566738e-01
```

Out[27]:		VIP	hoggorm pls	sMC hoggorm pls	IPW sklearn Ridge
	CRIM		7	5	8
	ZN		3	7	5
	INDUS		6	1	11
	CHAS		12	10	12
	NOX		13	2	13
	RM		10	9	10
	AGE		4	3	4
	DIS		11	13	9
	RAD		8	12	6
	TAX		1	11	1
	PTRATIO		9	8	7
	В		2	4	2
	LSTAT		5	6	3

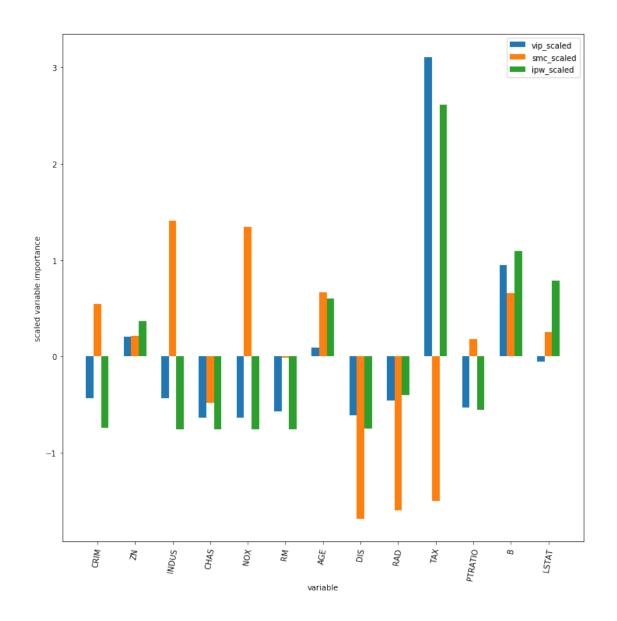
# 1.4.3 Visulization

Scaling



# histogram

```
In [55]: plt.figure(figsize=(12,12))
    w = 0.2
    plt.bar(np.arange(len(vip_scaled))-w, vip_scaled,width=w, label ='vip_scaled')
    plt.bar(np.arange(len(smc_scaled)), smc_scaled,width=w, label ='smc_scaled')
    plt.bar(np.arange(len(ipw_scaled))+w, ipw_scaled,width=w, label ='ipw_scaled')
    plt.xticks(range(X.shape[1]), data['feature_names'], rotation=80)
    plt.yticks(size=10)
    plt.legend(loc='upper right')
    plt.xlabel('variable')
    plt.ylabel('scaled variable importance')
    plt.show()
```



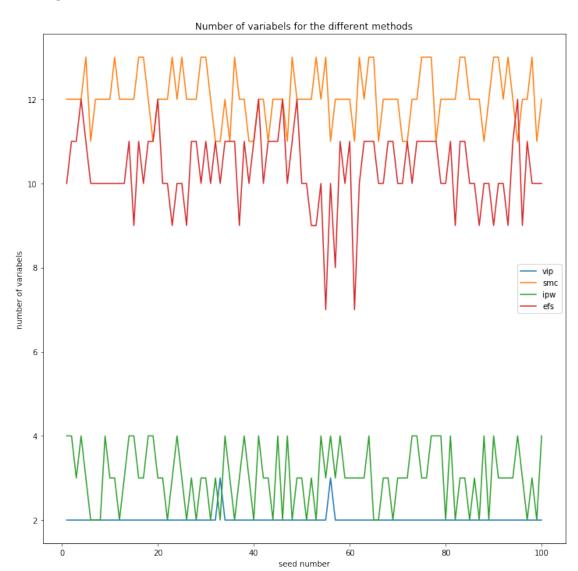
# 1.5 Effects on Key Peformance Indicators

```
Features: 8191/8191
Out[311]: ExhaustiveFeatureSelector(clone_estimator=True, cv=5,
                       estimator=Ridge(alpha=1.0, copy_X=True, fit_intercept=True, max_iter=No:
             normalize=False, random_state=None, solver='auto', tol=0.001),
                       max_features=13, min_features=1, n_jobs=1,
                       pre_dispatch='2*n_jobs', print_progress=True,
                       scoring='neg_mean_absolute_error')
In [ ]: ## introducing efs
        r1 = Ridge()
        efs1 = EFS(r1,
                   min_features=1,
                   max_features=13,
                   scoring='mean_absolute_error'#'neg_mean_squared_error',
                   print_progress=True,
                   cv=5)
        ## Models
        baseline = Ridge()
        vip_model = Ridge()
        smc_model = Ridge()
        ipw_model = Ridge()
        r_efs = Ridge()
        r = Ridge() # for readability used inside the IPW
        ## score storage
        baseline_scores = []
        vip_scores = []
        smc_scores = []
        ipw_scores = []
        efs_score = []
        ## number of parameters storage
        no_param_vip = []
        no_param_smc = []
        no_param_ipw = []
        no_param_efs = []
        ## time consumption storage
        time_vip = []
        time_smc = []
        time_ipw = []
        efs_times = []
        storage = {}
        for state in range(100):
```

```
X_train, X_test, y_train, y_test = train_test_split(X,
                                                    test_size=0.3,
                                                    random_state=state)
pls = ho.nipalsPLS1(X_train, y_train.reshape(np.shape(y_train)[0],1), cvType=['loo
vip = VIP()
smc = sMC()
ipw = IPW()
#time fit_tranform efs
t0_efs1 = time.time()
efs1.fit(X_train, y_train)
t1_efs1 = time.time()
efs_times.append(t1_efs1-t0_efs1)
#time fit_tranform vip
t0 = time.time()
vip_trans = vip.fit_transform(pls,X_train,threshold=1)
t1 = time.time()
time_vip.append(t1-t0)
#time fit_tranform smc
t0 = time.time()
smc_trans = smc.fit_transform(pls, X_train, alpha_mc=0.001)
t1 = time.time()
time\_smc.append(t1-t0)
#time fit_tranform IPW
t0 = time.time()
ipw_trans = ipw.fit_transform(r,X_train,y_train,no_iter=40,threshold=0.05)
t1 = time.time()
time_ipw.append(t1-t0)
#Storage of number of parameters
no_param_vip.append(np.shape(vip_trans)[1])
no_param_smc.append(np.shape(smc_trans)[1])
no_param_ipw.append(np.shape(ipw_trans)[1])
no_param_efs.append(len(efs1.best_idx_))
#transform test data
vip_test = vip.transform(X_test,threshold=1)
smc_test = smc.transform(X_test)
ipw_test = ipw.transform(X_test)
#fit different models to given data
baseline.fit(X_train,y_train)
vip_model.fit(vip_trans,y_train)
```

```
smc_model.fit(smc_trans,y_train)
            ipw_model.fit(ipw_trans,y_train)
            r_efs.fit(X_train[:,efs1.best_idx_],y_train)
            storage[str(state)] = data['feature_names'][vip.importances>1]
            baseline_scores.append(mean_absolute_error(y_test, baseline.predict(X_test)))
            vip_scores.append(mean_absolute_error(y_test,vip_model.predict(vip_test)))
            smc_scores.append(mean_absolute_error(y_test,smc_model.predict(smc_test)))
            ipw_scores.append(mean_absolute_error(y_test,ipw_model.predict(ipw_test)))
            efs score.append(mean_absolute_error(y_test, r_efs.predict(X_test[:,efs1.best_idx_
In [296]: print('
                     avrage mean squared error for baseline model is {0:4f} with std +/-{1:4f}
                     avrage mean squared error for vip selection is \{0:4f\} with std +/-\{1:4f\}'
          print('
                     avrage mean squared error for smc selection is \{0:4f\} with std +/-\{1:4f\}'
          print('
                     avrage mean squared error for ipw selection is \{0:4f\} with std +/-\{1:4f\}'
          print('
          print('
                     avrage mean squared error for efs model is {0:4f} with std +/-{1:4f}'.for
    avrage mean squared error for baseline model is 8.264785 with std +/-3.701695
    avrage mean squared error for vip selection is 5.861383 with std +/-0.379991
    avrage mean squared error for smc selection is 7.227898 with std +/-3.752635
    avrage mean squared error for ipw selection is 6.045653 with std +/-0.650087
    avrage mean squared error for baseline model is 3.453203 with std +/-0.244792
In [304]: col_names= ['Average mse', 'Standard deviation', 'Average number of features', 'average
          KPI = pd.DataFrame(index =col_names)
          KPI['Baseline'] = pd.Series([np.mean(baseline_scores),np.std(baseline_scores),13,0],
          KPI['VIP'] = pd.Series([np.mean(vip_scores),np.std(vip_scores),np.mean(no_param_vip)
          KPI['sMC'] = pd.Series([np.mean(smc_scores),np.std(smc_scores),np.mean(no_param_smc)
          KPI['IPW'] = pd.Series([np.mean(ipw_scores),np.std(ipw_scores),np.mean(no_param_ipw)
          KPI['EFS'] = pd.Series([np.mean(efs_score),np.std(efs_score),np.mean(no_param_efs),np.mean(no_param_efs),np.mean(no_param_efs)
          KPI
Out [304]:
                                                       VIP
                                                                             IPW \
                                        Baseline
                                                                   \mathsf{sMC}
          Average mse
                                        8.264785 5.861383
                                                             7.227898
                                                                       6.045653
          Standard deviation
                                        3.701695 0.379991
                                                             3.752635
                                                                       0.650087
          Average number of features 13.000000 2.020000 12.060000
                                                                        3.020000
          average time fit_transform
                                        0.000000 0.000210
                                                            0.000791 0.025638
                                             EFS
                                        3.453203
          Average mse
          Standard deviation
                                        0.244792
          Average number of features 10.310000
          average time fit_transform 54.709215
In [247]: plt.figure(figsize=(12,12))
          plt.plot(range(1,101),no_param_vip,label='vip')
          plt.plot(range(1,101),no_param_smc,label='smc')
```

```
plt.plot(range(1,101),no_param_ipw,label='ipw')
plt.plot(range(1,101),no_param_efs,label='efs')
plt.legend(loc='best')
plt.xlabel('seed number')
plt.ylabel('number of variabels')
plt.title('Number of variabels for the different methods')
plt.show()
```



# 1.5.1 Output from the different PLS algorithms