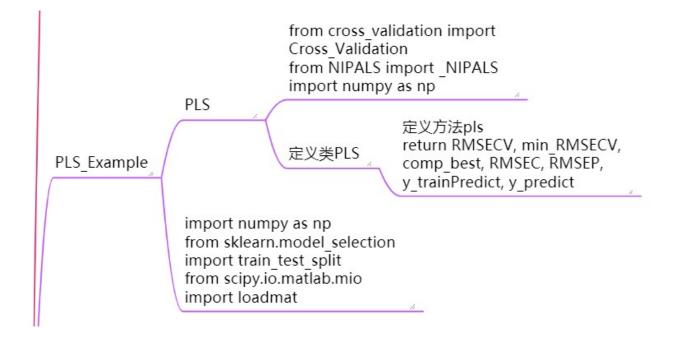
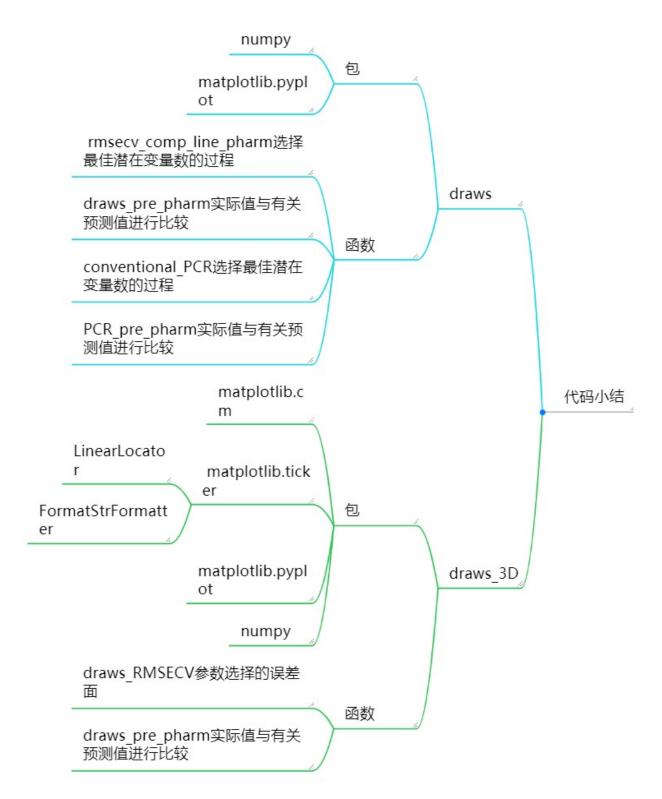
## PLS\_Example

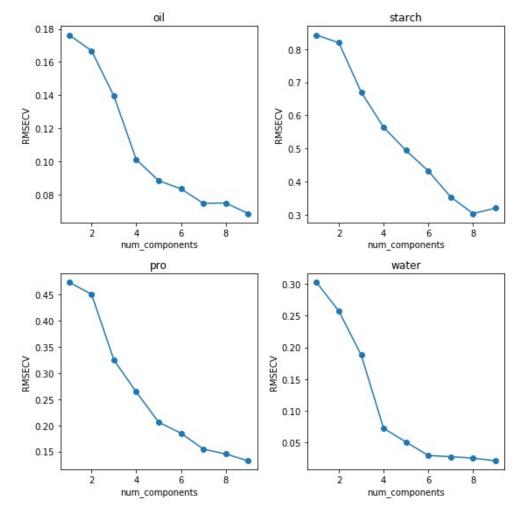




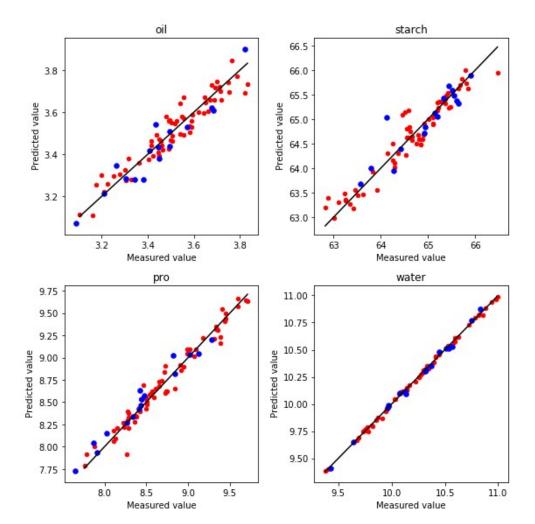
```
In [3]: import numpy as np
    from sklearn.model_selection import train_test_split
    from scipy.io.matlab.mio import loadmat
    from PLS import PLS
    from draws import rmsecv_comp_line_pharm,draws_pre_pharm
```

```
In [2]: if __name__ == '__main__':
            fname = loadmat('E:\Documents\DAY\cornmat.mat')
            #print fname.keys()
            X = ('m5', 'mp5', 'mp6')
            Y = ('oil', 'starch', 'pro', 'water')
            for a in X: #对每个instrument
                rmsecv list = []
                Y \text{ test} = []
                Y predict = []
                Y trainPredict = []
                Y train = []
                for b in Y:
                    x = fname[a]
                    y = fname[b][:, 0:1]
                    #print x.shape, y.shape
                    x_train, x_test, y_train, y_test = train_test_split(x, y, test_size=
        0.2, random state=0)
                    demo = PLS(x train, y train, x test, y test, n fold=10, max componen
        ts=9)
                    RMSECV, min RMSECV, comp best, RMSEC, RMSEP, y trainPredict, y predi
        ct = demo.pls()
                    rmsecv_list.append(RMSECV)
                    Y test.append(np.squeeze(y test).tolist())#数组降维并转换为list
                    Y_predict.append(np.squeeze(y_predict).tolist())
                    Y_trainPredict.append(np.squeeze(y_trainPredict).tolist())
                    Y train.append(np.squeeze(y train).tolist())
                    print a,b
                    print 'RMSECV', RMSECV
                    print 'min RMSECV', min RMSECV
                    print 'comp_best', comp_best
                    print 'RMSEP:', RMSEP
                    print '\n'
                print "The selection process of the optimal latent variables number from
        PLS model about the ",a
                rmsecv_comp_line_pharm(9, rmsecv_list)
                print "The actual value compared with the predicted value about the ",
        a," instrument."
                draws_pre_pharm(Y_test, Y_predict, Y_trainPredict, Y_train)
```

```
m5 oil
RMSECV [ 0.17629096  0.16681719  0.13940448  0.10102171  0.08829704  0.0833613
 0.07462155 0.07482885 0.06846579]
min RMSECV 0.0684657921342
comp_best 9
RMSEP: [ 0.06048119]
m5 starch
0.30304482 0.3191829 ]
min RMSECV 0.303044815403
comp best 8
RMSEP: [ 0.28423622]
m5 pro
RMSECV [ 0.47366436  0.45083695  0.32488889  0.26400453  0.20601404  0.1849906
 0.15457974 0.14524952 0.13223247]
min RMSECV 0.132232472901
comp best 9
RMSEP: [ 0.1028038]
m5 water
RMSECV [ 0.30269952  0.25737487  0.18808281  0.072574  0.05098757  0.0296102
 0.02774756 0.02554763 0.02129437]
min RMSECV 0.0212943734628
comp best 9
RMSEP: [ 0.0238987]
```

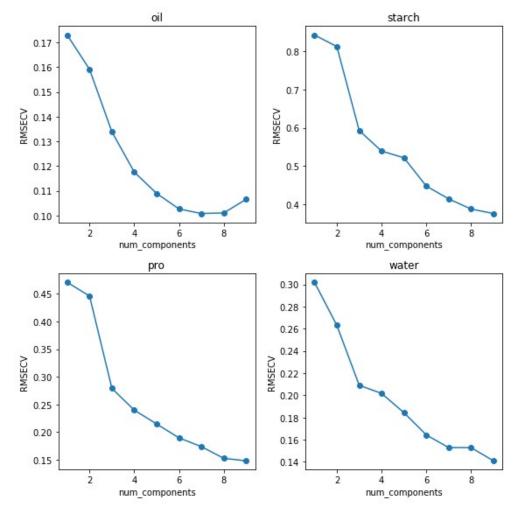


The actual value compared with the predicted value about the m5 instrument.

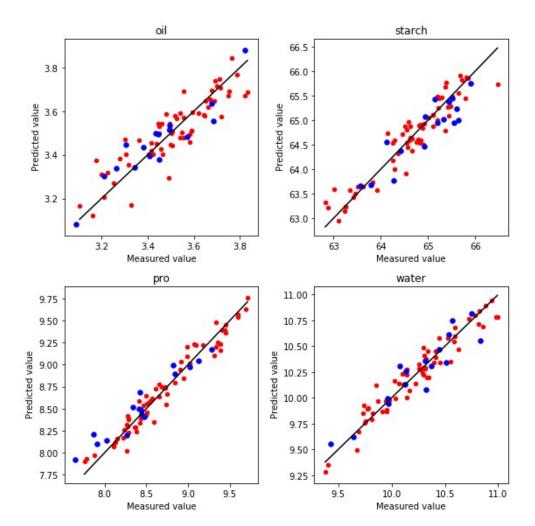


```
mp5 oil
RMSECV [ 0.17305513  0.15916037  0.13384274  0.11755294  0.10892071  0.1026341
 0.10078927 0.10102846 0.10654359]
min RMSECV 0.100789270821
comp_best 7
RMSEP: [ 0.07055259]
mp5 starch
RMSECV [ 0.84306041  0.81294549  0.59268484  0.53894313  0.52135504  0.447189
 0.41362547 0.38701688 0.37524013]
min RMSECV 0.375240126108
comp best 9
RMSEP: [ 0.34004861]
mp5 pro
RMSECV [ 0.47075969  0.44586737  0.27886217  0.2396058  0.21453646  0.1894598
 0.17352615 0.1524408 0.14797374]
min RMSECV 0.147973741433
comp best 9
RMSEP: [ 0.16101876]
mp5 water
RMSECV [ 0.30187712  0.26307321  0.20904577  0.20171082  0.18436796  0.1643146
 0.15284302 0.15286832 0.14095779]
min RMSECV 0.14095778542
comp best 9
RMSEP: [ 0.13670961]
```

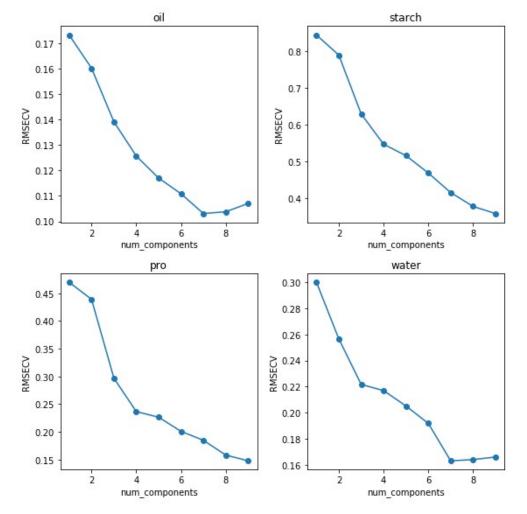
The selection process of the optimal latent variables number from PLS model ab out the  $\mbox{\em mp5}$ 



The actual value compared with the predicted value about the mp5 instrument.



```
mp6 oil
RMSECV [ 0.17331899  0.16023794  0.13914462  0.12570084  0.11702873  0.1108517
0.10308057 0.10376007 0.10706935]
min RMSECV 0.103080572518
comp_best 7
RMSEP: [ 0.07013598]
mp6 starch
RMSECV [ 0.84374778  0.78911515  0.62904305  0.54680608  0.51579505  0.4684237
 0.41528782 0.37768861 0.35826078]
min RMSECV 0.358260775913
comp best 9
RMSEP: [ 0.31259899]
mp6 pro
RMSECV [ 0.46988772  0.43916345  0.29678658  0.23660799  0.22643758  0.2009111
 0.18487403 0.15813341 0.14781656]
min RMSECV 0.147816560997
comp best 9
RMSEP: [ 0.14034578]
mp6 water
0.16315016 0.1640678 0.16602371]
min RMSECV 0.163150159884
comp best 7
RMSEP: [ 0.15609604]
```



The actual value compared with the predicted value about the mp6 instrument.

