
```

clear all; close all; clc
load('Inorfull.mat')

for i=1:26
    DATA1(i,:)=DATA(5*(i-1)+1,:);           % select 1st of each blocks
    CONC1(i,:)=CONC(5*(i-1)+1,:);           % select 1st of each blocks
end
Z=DATA1';                                     % data matrix 176x26
[u,s,v]=svd(Z);                             % svd

for k=1:176
    RMSE(k)=0;

    for i=1:26
        s1=s(1:k,:);                         % kx26
        u1=u(:,1:k);                         % 26xk
        T=s1*v';                             % kx26
        T1=T;
        T1(:,i)=[];                         % leave ith score out kx25

        conc=CONC1;
        conc(i,:)=[];                       % leave ith conc out, 25x3
        P=[PureCo; PureCr; PureNi];
        Y=(P'*conc)';                       % dependent quantity of OLS
        regression (176x3)(3x25)=176x25
        B=T1'\Y;                             % Regression matrix Y=T1'B 25x176=(25xk)
        (kx176)

        c_p=T(:,i)'\*B*P'\*inv(P*P');        % predicted concentration

        RMSE(k)=RMSE(k)+norm(c_p-CONC1(i,:));

    end
end

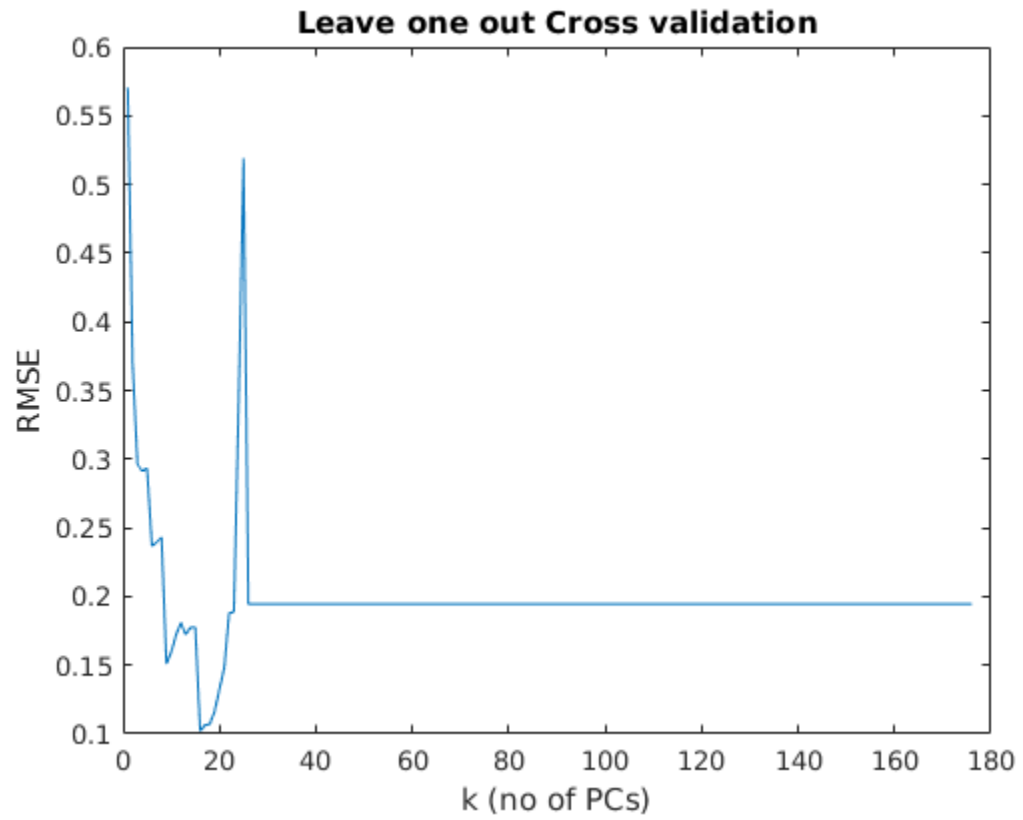
[M,m]=min(RMSE);
fprintf('\n\n-----\n\n')
fprintf('\n Number of PCs is %d \n',m)
fprintf('\n RMSE=%d \n',M)
fprintf('\n\n-----\n\n')
plot([1:176],RMSE)
xlabel('k (no of PCs)')
ylabel('RMSE')
title('Leave one out Cross validation')

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Number of PCs is 16

```

$RMSE=1.019814e-01$



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