

PLS Mean Centering

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Partial Least Squares (PLS) with Mean Centering

Partial least squares usually uses mean-centered data to compute C_{pls} using the weights from the SIMPLS algorithm with r latent variables.

```
X = A_train;
Y = C_train;

X0 = X - mean(X,1);
Y0 = Y - mean(Y,1);
[X_loadings, Y_loadings, X_scores, Y_scores, Weights] = pnnl_simpls(X0, Y0, r);

B_pls = Weights * Y_loadings';

C_pls = (A_unknown - mean(A_train,1)) * B_pls + mean(C_train,1);
```

Partial Least Squares (PLS) without Mean Centering

The following is PLS without mean centering.

```
X = A_train;
Y = C_train;

[X_loadings, Y_loadings, X_scores, Y_scores, Weights] = pnnl_simpls(X, Y, r);

B_pls = Weights * Y_loadings';

C_pls = A_unknown * B_pls;
```

Combined algorithm

To make it easier to run with the rest of the tools in the PNNL toolbox, we combined mean-centered and non-mean-centered into one function with meanCentered as an optional argument. When meanCentered is not used as an input, then the default is to compute without mean-centered data.

```
function [C_pls, B_pls] = pnnl_pls(A_train, C_train, A_unknown, r, meanCentered)
    if nargin < 5
        meanCentered = false;
    end

    X = A_train;
    Y = C_train;
    if meanCentered
        X0 = X - mean(X,1);
        Y0 = Y - mean(Y,1);
    else
        X0 = X;
        Y0 = Y;
    end

    [X_loadings, Y_loadings, X_scores, Y_scores, Weights] = pnnl_simpls(X0, Y0, r); %#ok<ASGLU>
```

```

B_pls = Weights * Y_loadings';

if meanCentered
    C_pls = (A_unknown - mean(A_train,1)) * B_pls + mean(C_train,1);
else
    C_pls = A_unknown * B_pls;
end
end

```

Napalm Data

Load the included napalm data to run the PLS algorithms.

```

clearvars
load pnnl_napalm_data
whos

```

Name	Size	Bytes	Class	Attributes
A_train	20x1713	274080	double	
A_unknown	12x1713	164448	double	
C_train	20x3	480	double	
C_validation	12x3	288	double	
ConcentrationUnits	1x4	8	char	
ConstituentNames	1x3	364	cell	
WavenumberLabel	1x20	40	char	
Wavenumbers	1x1713	13704	double	

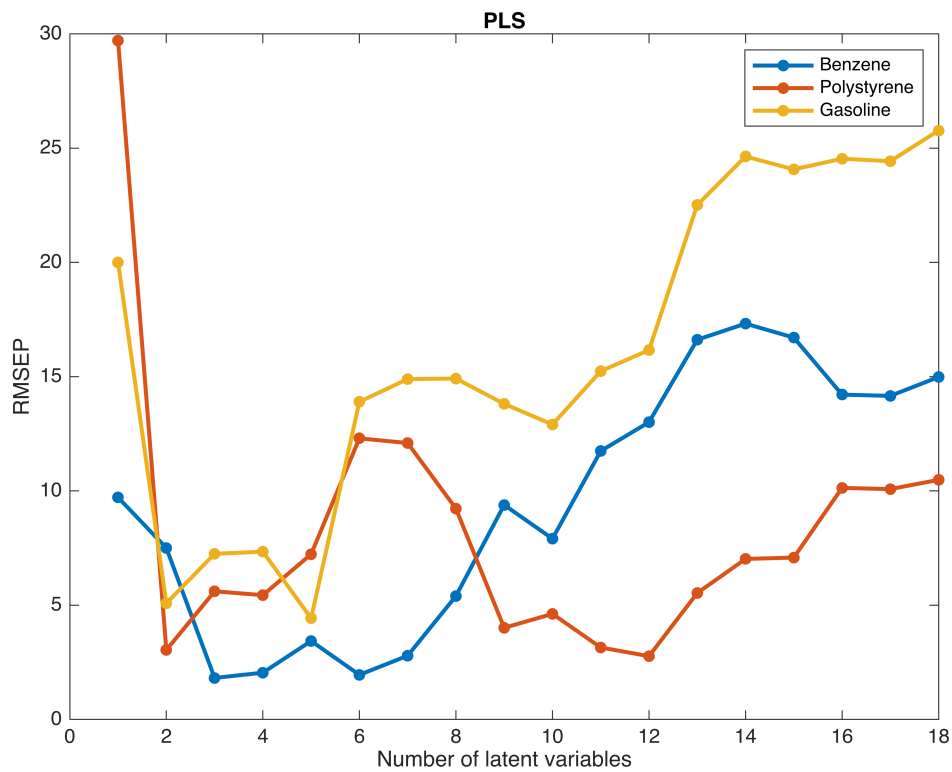
Optimal number of latent variables for PLS with mean centering

Compute PLS with mean centering for 1 through 18 latent variables and plot RMSEP for them.

```

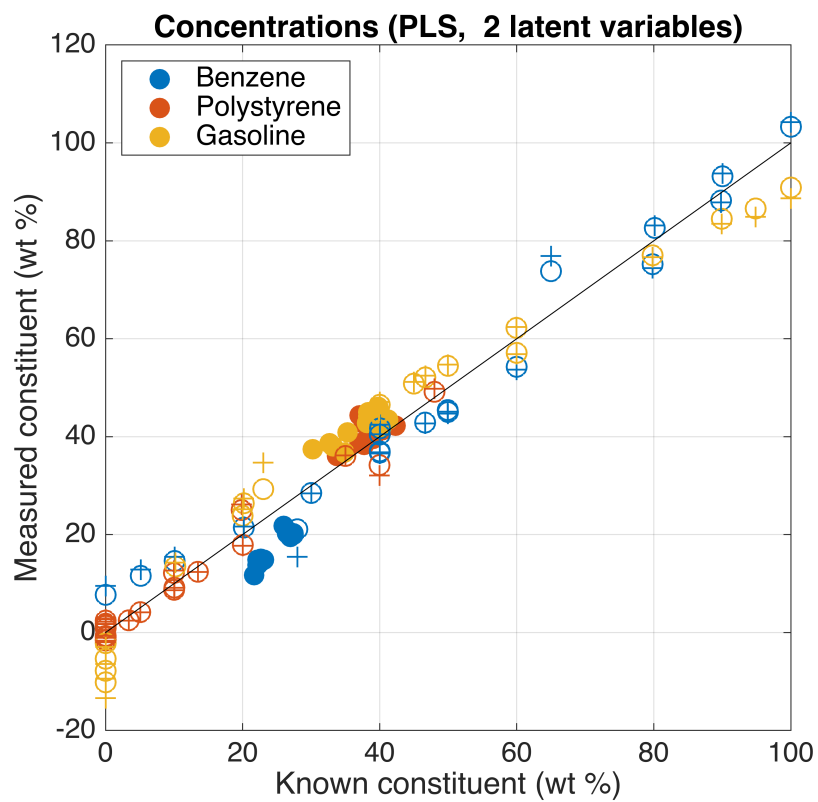
nLatentVariables = 1:18;
meanCentered = true;
[C_pls, RMSEP_pls] = pnnl_napalm_pls(nLatentVariables,meanCentered);
plot(nLatentVariables, RMSEP_pls,'.-','LineWidth',2,'MarkerSize',20)
xlabel('Number of latent variables')
ylabel('RMSEP')
title('PLS')
legend(ConstituentNames{:})

```



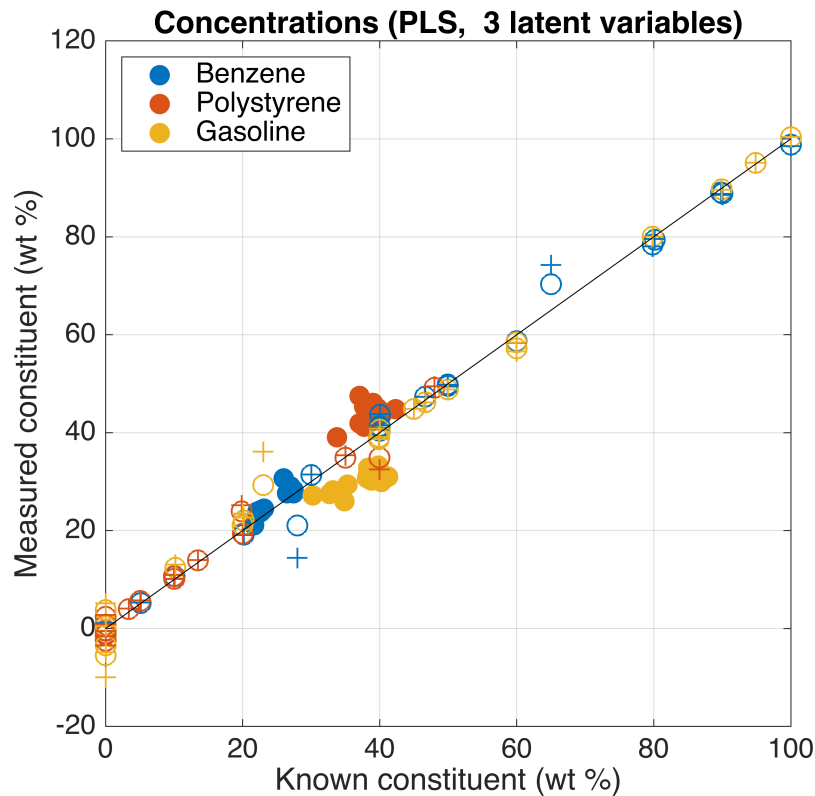
For mean-centered data, it looks like the knee in the curve for polystyrene and gasoline is 2 latent variables, and 3 for benzene. Plot them to see what they look like.

```
nLatentVariables = [2,3];  
pnnl_napalm_pls(nLatentVariables,meanCentered);
```



Legend: Dot is predicted. Circle is train. Cross is cross-validation.

PLS, 2 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	4.5616	2.2064	5.8133
RMSECV	5.8788	2.7588	7.2286
RMSEP	7.5077	3.04	5.0846



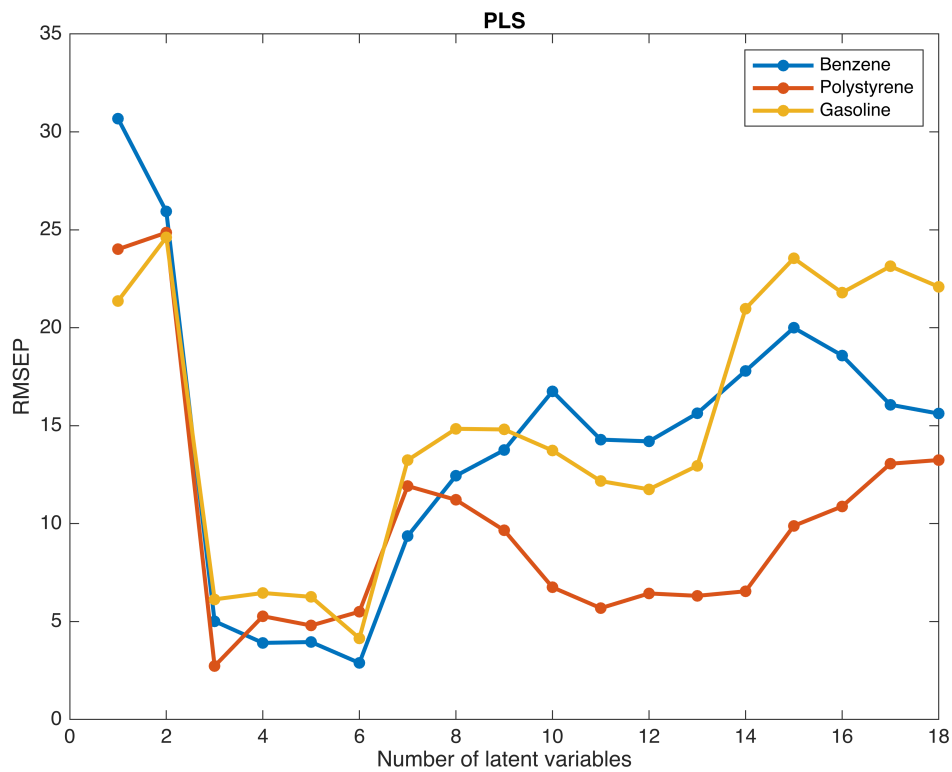
Legend: Dot is predicted. Circle is train. Cross is cross-validation.

PLS, 3 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	2.2847	1.7662	2.4538
RMSECV	3.9022	2.4136	4.2785
RMSEP	1.8185	5.6092	7.2521

Optimal number of latent variables for PLS without mean centering

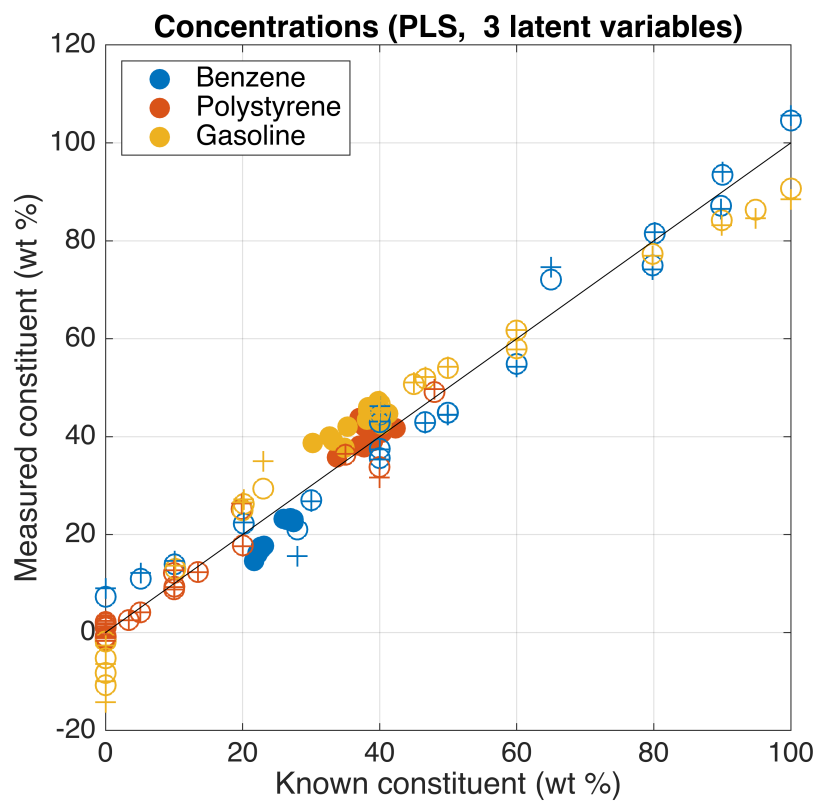
Compute PLS without mean centering for 1 through 18 latent variables and plot RMSEP for them.

```
nLatentVariables = 1:18;
meanCentered = false;
[C_pls, RMSEP_pls] = pnnl_napalm_pls(nLatentVariables,meanCentered);
plot(nLatentVariables, RMSEP_pls,'.-','LineWidth',2,'MarkerSize',20)
xlabel('Number of latent variables')
ylabel('RMSEP')
title('PLS')
legend(ConstituentNames{:})
```



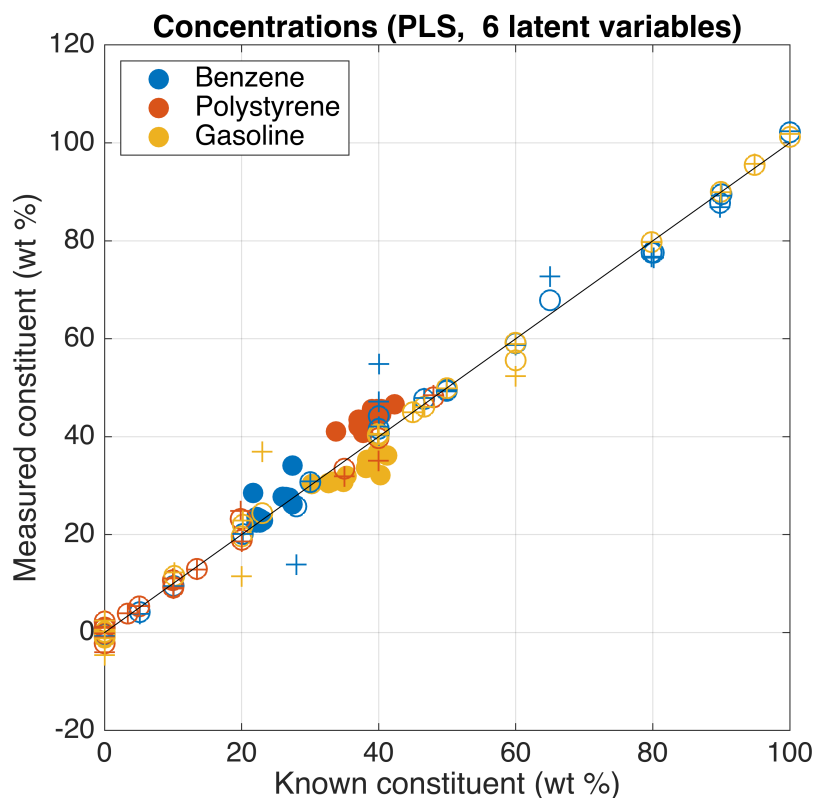
Without mean centering, it looks like the knee in the curve for polystyrene is 3 latent variables and 6 for benzene and gasoline. Plot them to see what they look like.

```
nLatentVariables = [3 6];
pnnl_napalm_pls(nLatentVariables,meanCentered);
```



Legend: Dot is predicted. Circle is train. Cross is cross-validation.

PLS, 3 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	4.6039	2.2753	5.923
RMSECV	5.8822	2.8386	7.4067
RMSEP	5.0162	2.7261	6.133



Legend: Dot is predicted. Circle is train. Cross is cross-validation.

PLS, 6 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	1.7183	1.2299	1.2676
RMSECV	5.377	2.1378	4.3161
RMSEP	2.8856	5.5043	4.1457

%#ok<ASGLU>

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