

# 2.160 Identification, Estimation, and Learning

## Part 1 Regression

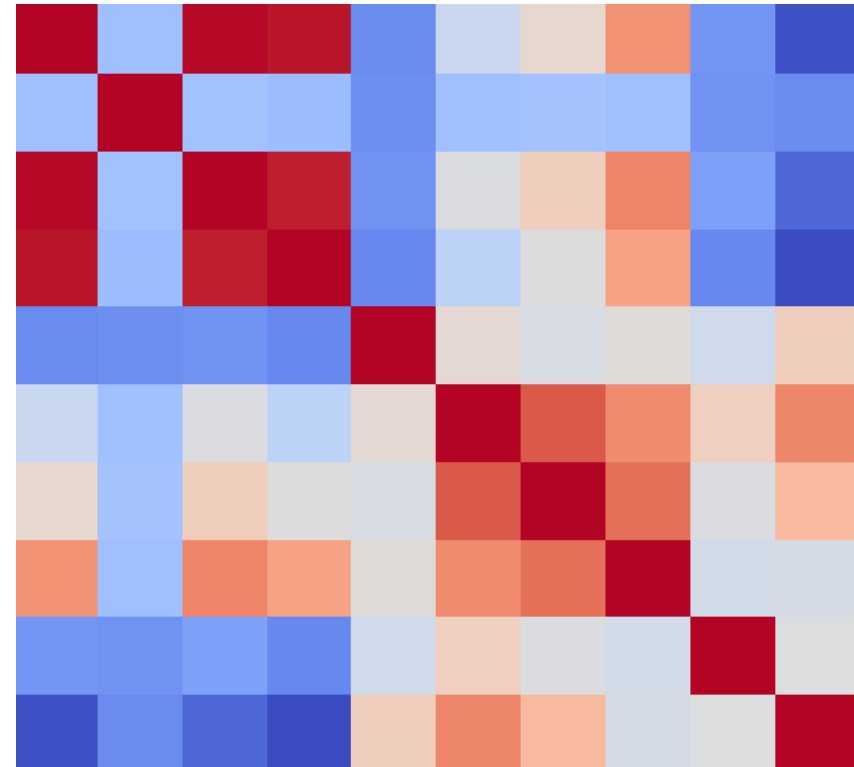
### Lecture 6

### Partial Least Squares Regression

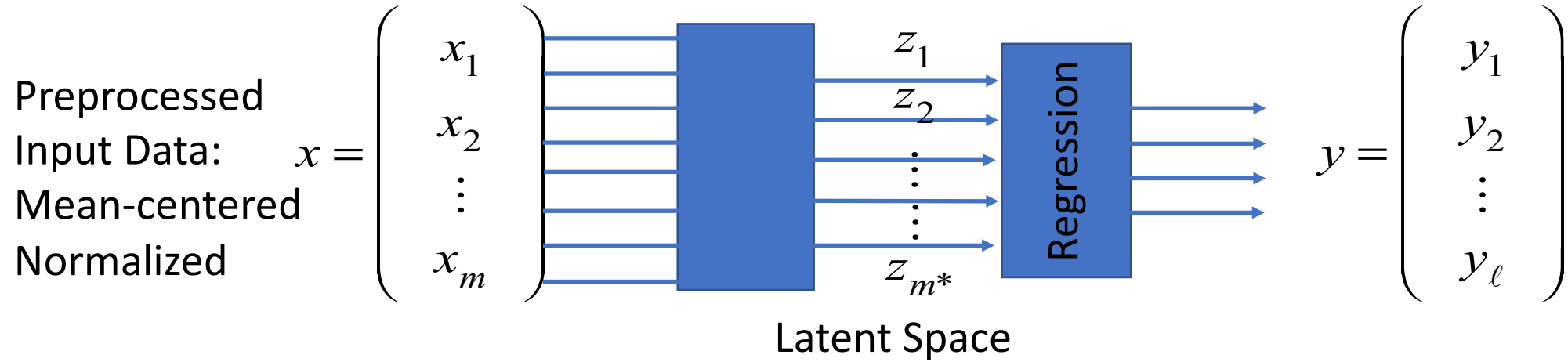
H. Harry Asada

Department of Mechanical Engineering

MIT

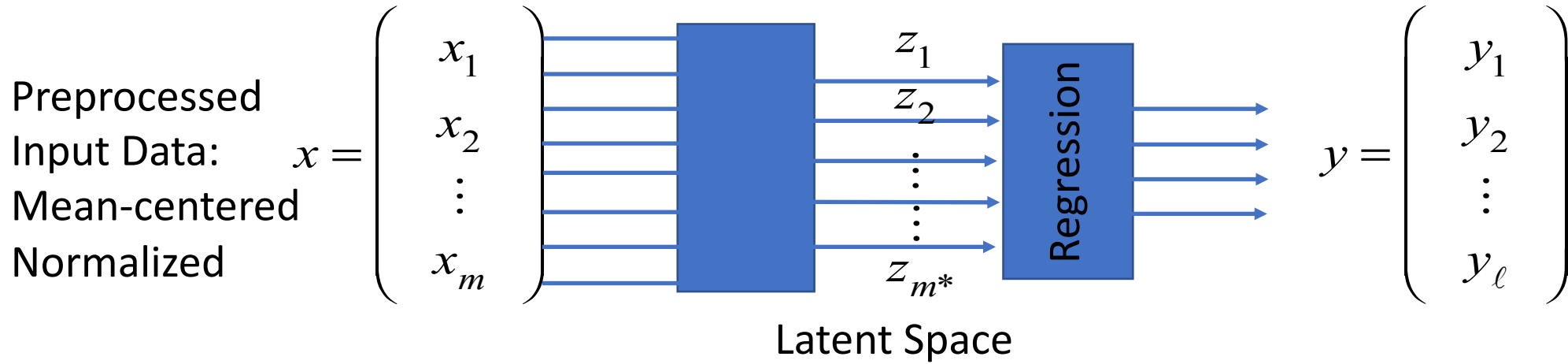


# Latent Modeling

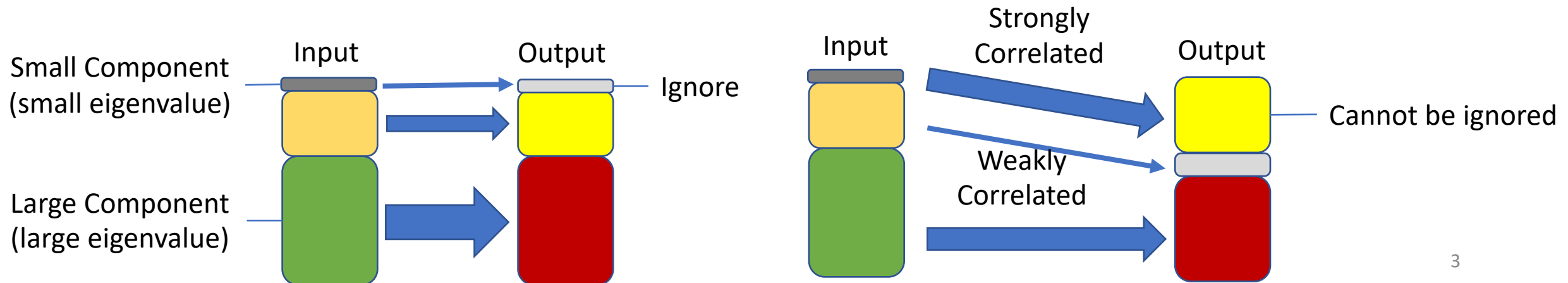


- ❑ Principal Component Regression: Characterizes the input data space, reduces the input dimension based on Principal Component Analysis, and regresses on principal components.

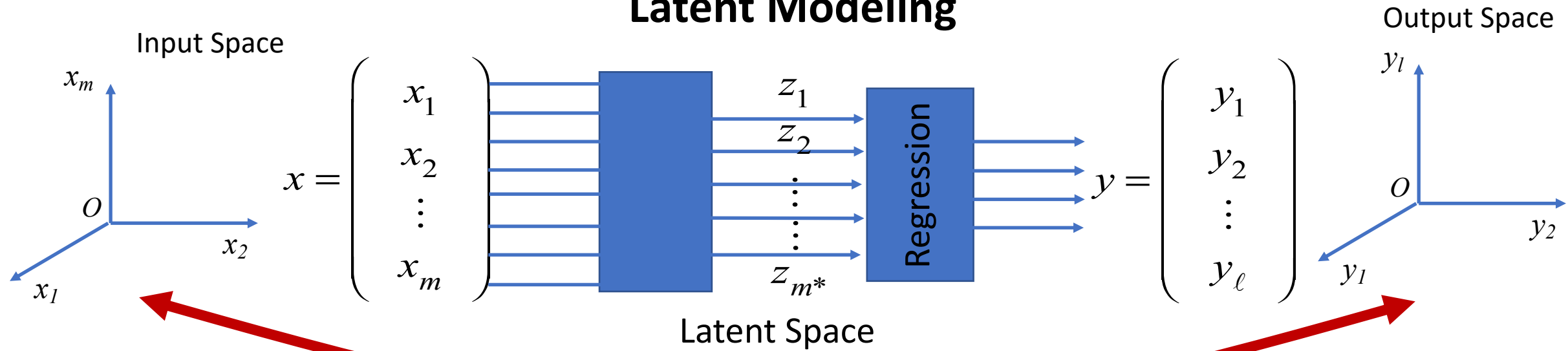
# Latent Modeling



- ❑ Principal Component Regression: Characterizes the input data space, reduces the input dimension based on Principal Component Analysis, and regresses on principal components.
- ❑ Caveat! Small principal components, which are ignored, may be highly correlated with outputs. Those components must not be neglected.



# Latent Modeling

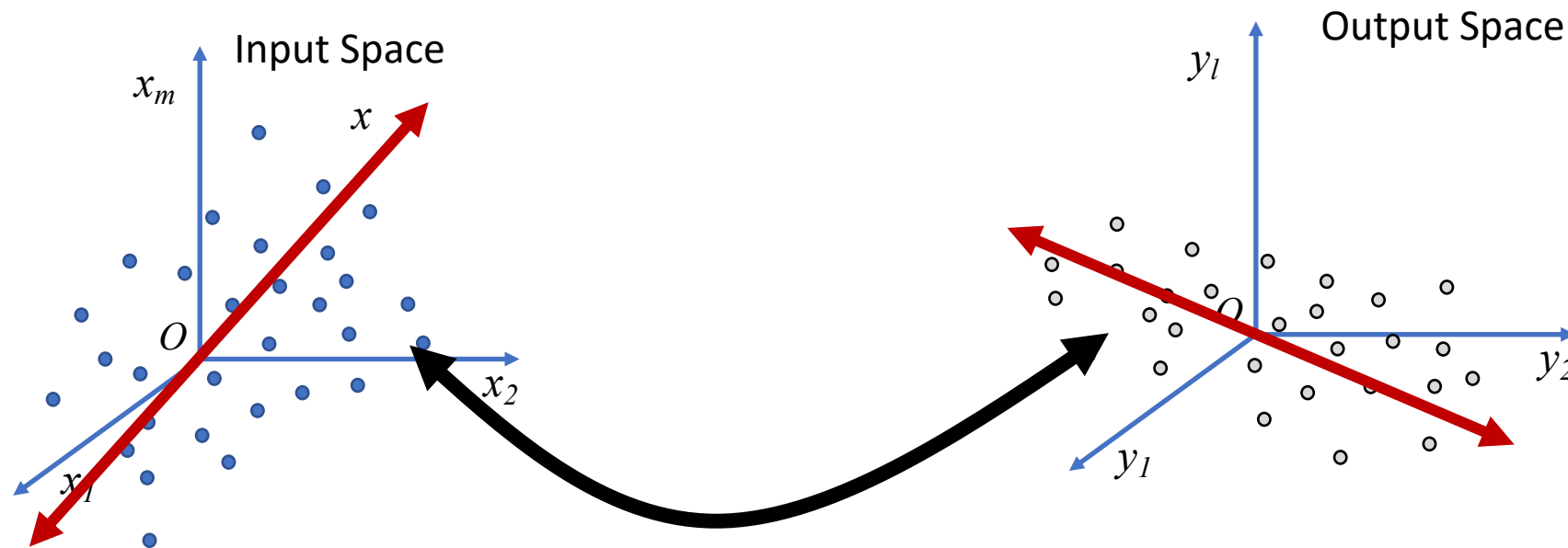


- ❑ Principal Component Regression. Characterizes the input data space, reduces the input dimension based on Principal Component Analysis, and uses the principal components.
- ❑ Caveat! Small principal components, which have low variance, may be highly correlated with outputs. Those components must not be neglected.
- ❑ Components having significant correlation with outputs must be involved in the latent space.
- ❑ This requires to analyze both input and output spaces, rather than characterizing the input space alone.
- ❑ Multiple Outputs: Unlike single output regressions, we often need to estimate multiple outputs, which may be correlated.
- ❑ This lecture will discuss the latent space modeling based on input – output correlation analysis.



## 4.3 The Core Algorithm of Multi-Input, Multi-Output Partial Least Squares Regression

Partial Least Squares Regression is a latent modeling method for predicting a set of outputs in relation to a reduced order inputs. The basic idea is to find a low-dimensional set of input space variables that is most correlated with a given set of output data. It is to analyze data in both input space and output space.



## 4.3 The Core Algorithm of Multi-Input, Multi-Output Partial Least Squares Regression

Step 1. Find the directions of a pair of unit vectors,  $v \in \mathbb{R}^m$  in the input space and  $w \in \mathbb{R}^\ell$  in the output space, that maximizes the correlation between the projection of input vector onto the unit vector,  $z = v^T x$ , and that of the output vector,  $r = w^T y$ .

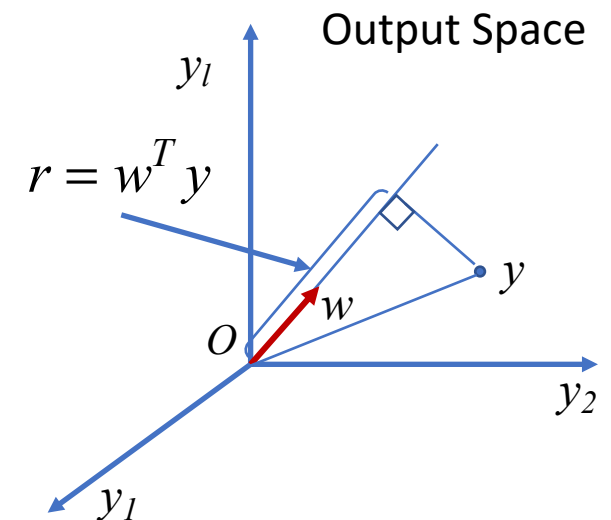
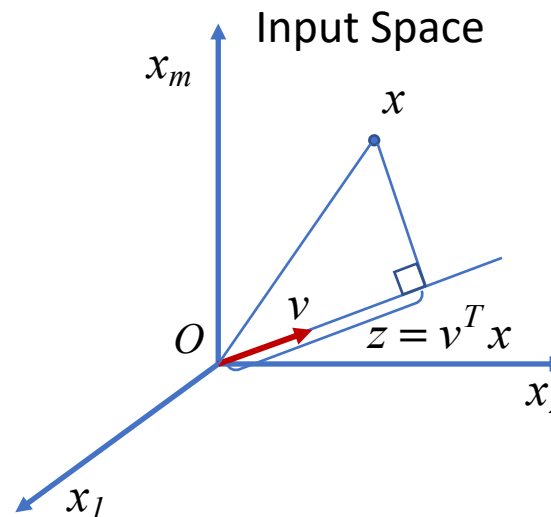
$$\max_{v,w} E[z \cdot r] = \max_{v,w} E[v^T x \cdot w^T y]$$

$$= \max_{v,w} v^T \underbrace{E[x y^T]}_{C_{XY}} w$$

where

$$|v| = 1, |w| = 1$$

Covariance of mean-centered random variables  $x$  and  $y$ .



□  $z = v^T x$  is called the **score** of input  $x$  with respect to  $v$ , and  $r = w^T y$  is called the **score** of output  $y$  with respect to  $w$ .

## Recap: Covariance Matrix

$$C_{XY} = E[x y^T] = E \left[ \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix} \begin{pmatrix} y_1 & \cdots & y_\ell \end{pmatrix} \right] = \begin{pmatrix} E[x_1 y_1] & \cdots & E[x_1 y_\ell] \\ \vdots & \ddots & \vdots \\ E[x_m y_1] & \cdots & E[x_m y_\ell] \end{pmatrix}$$

Note  $x$  and  $y$  are mean-centered and normalized.

Problem

$$\max_{v, w} v^T C_{XY} w \quad \text{Subject to} \quad |v| = 1, |w| = 1$$

**Solution:** Using two Lagrange multipliers for the two constraint equations,

$$(v^o, w^o) = \arg \max_{v, w} \left\{ v^T C_{XY} w - \underbrace{\frac{1}{2} \lambda_v (v^T v - 1) - \frac{1}{2} \lambda_w (w^T w - 1)}_{\text{2 Constraints}} \right\}$$

2 Constraints

A function of both  $v$  and  $w$

**Solution:** Using two Lagrange multipliers,

$$(v^o, w^o) = \arg \max_{v, w} \left\{ v^T C_{XY} w - \frac{1}{2} \lambda_v (v^T v - 1) - \frac{1}{2} \lambda_w (w^T w - 1) \right\}$$

The necessary conditions for  $v$  and  $w$  to maximize the correlation are:

$$\frac{\partial}{\partial v} = 0 \Rightarrow C_{XY} w - \lambda_v v = 0 \quad (35)$$

$$\frac{\partial}{\partial w} = 0 \Rightarrow (C_{XY})^T v - \lambda_w w = 0 \quad (36)$$

Note that by definition:  $(C_{XY})^T = C_{YX}$ .

## Quick clarification: Transpose of a Covariance Matrix

$$\begin{aligned}
 (C_{XY})^T &= \begin{pmatrix} E[x_1 y_1] & \cdots & E[x_1 y_\ell] \\ \vdots & \ddots & \vdots \\ E[x_m y_1] & \cdots & E[x_m y_\ell] \end{pmatrix}^T = \begin{pmatrix} E[x_1 y_1] & \cdots & E[x_m y_1] \\ \vdots & \ddots & \vdots \\ E[x_1 y_\ell] & \cdots & E[x_m y_\ell] \end{pmatrix} \\
 &= \begin{pmatrix} E[y_1 x_1] & \cdots & E[y_1 x_m] \\ \vdots & \ddots & \vdots \\ E[y_\ell x_1] & \cdots & E[y_\ell x_m] \end{pmatrix} = E \left( \begin{pmatrix} y_1 \\ \vdots \\ y_\ell \end{pmatrix} \begin{pmatrix} x_1 & \cdots & x_m \end{pmatrix} \right) = C_{YX}
 \end{aligned}$$

Or, simply

$$\left( \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix} \begin{pmatrix} y_1 & \cdots & y_\ell \end{pmatrix} \right)^T = \begin{pmatrix} y_1 & \cdots & y_\ell \end{pmatrix}^T \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix}^T = \begin{pmatrix} y_1 \\ \vdots \\ y_\ell \end{pmatrix} \begin{pmatrix} x_1 & \cdots & x_m \end{pmatrix}$$

**Solution:** Using Lagrange multipliers,

$$(v^o, w^o) = \arg \max_{v, w} \left\{ v^T C_{XY} w - \frac{1}{2} \lambda_v (v^T v - 1) - \frac{1}{2} \lambda_w (w^T w - 1) \right\}$$

The necessary conditions for  $v$  and  $w$  to maximize the correlation are:

$$\frac{\partial}{\partial v} = 0 \Rightarrow C_{XY} w - \lambda_v v = 0 \quad (35) \qquad \frac{\partial}{\partial w} = 0 \Rightarrow (C_{XY})^T v - \lambda_w w = 0 \quad (36)$$

Note that by definition:  $(C_{XY})^T = C_{YX}$ .

From (36),  $w = \frac{1}{\lambda_w} C_{YX} v$ . Substituting this in (35) yields.  $C_{XY} C_{YX} v = \lambda_v \lambda_w v$

This implies that vector  $v$  is an eigen vector of matrix  $C_{XY} C_{YX}$

Similarly, from (35)  $v = \frac{1}{\lambda_v} C_{XY} w$ . Substituting this into (36) yields  $C_{YX} C_{XY} w = \lambda_v \lambda_w w$

This implies that vector  $w$  is an eigen vector of matrix  $C_{YX} C_{XY}$

$$C_{XY}C_{YX}v = \lambda_v \lambda_w v$$

$$C_{YX}C_{XY}w = \lambda_v \lambda_w w$$

Note that in both cases the eigenvalue is the same :  $\lambda_v \lambda_w$

We can show that  $\lambda_v = \lambda_w$

Pre-multiplying  $v^T$  to (35),  $C_{XY}w - \lambda_v v = 0$

$$v^T C_{XY}w - \lambda_v v^T v = 0 \quad \therefore \lambda_v = v^T C_{XY}w$$

Pre-multiplying  $w^T$  to (36),  $(C_{YX})^T v - \lambda_w w = 0$

$$w^T (C_{XY})^T v - \lambda_w w^T w = 0 \quad \therefore \lambda_w = w^T (C_{XY})^T v = v^T (C_{XY}) w = \lambda_v$$

$$\therefore \lambda_v = \lambda_w$$

$C_{XY}C_{YX}$  and  $C_{YX}C_{XY}$  have the same eigenvalues.  $\lambda_v = \lambda_w = \lambda$



# Singular Value Decomposition --- Extension of Eigen Decomposition

A matrix  $A \in \mathbb{R}^{m \times \ell}$  can be decomposed to

$$A = VDW^T$$

where

$$V = \begin{bmatrix} v_1 & v_2 & \cdots & v_m \end{bmatrix} \in \mathbb{R}^{m \times m}$$

$v_i$  = the  $i$ -th left singular vector of matrix  $A$   
 = the eigenvectors of matrix  $AA^T \in \mathbb{R}^{m \times m}$ ,  
 which is a real, symmetric matrix having  
 all real eigenvalues and eigen vectors.

$$W = \begin{bmatrix} w_1 & w_2 & \cdots & w_m \end{bmatrix} \in \mathbb{R}^{\ell \times \ell}$$

$w_i$  = the  $i$ -th right singular vector of matrix  $A$   
 = the eigenvectors of matrix  $A^T A \in \mathbb{R}^{\ell \times \ell}$ ,  
 which is a real, symmetric matrix having  
 all real eigenvalues and eigen vectors.

$$D = \begin{pmatrix} s_1 & 0 & \cdots & 0 \\ 0 & s_2 & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & \cdots & s_\ell \\ 0 & \cdots & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & \cdots & \cdots & 0 \end{pmatrix} \in \mathbb{R}^{m \times \ell}$$

: a rectangular  
diagonal matrix

$s_i$  = the  $i$ -th singular value of matrix  $A$   
 = the square root of the non-zero eigenvalue  
 of matrix  $AA^T \in \mathbb{R}^{m \times m}$ , or  $A^T A \in \mathbb{R}^{\ell \times \ell}$ , both  
 are real-symmetric, positive semi-definite  
 matrices with non-negative eigenvalues.

# Theorem

The unit vectors,  $v_0$  and  $w_0$ , that maximize the correlation between input and output scores,  $z = v^T x$  and  $r = w^T y$ , are the left and right singular vectors, respectively, associated with the largest singular value of the cross-correlation matrix  $C_{XY}$ .

$$C_{XY} = \begin{bmatrix} \underline{v_1} & \dots & \dots \end{bmatrix} \begin{bmatrix} \underline{s_1} & \dots & 0 \\ \vdots & * & 0 \\ 0 & 0 & \dots \end{bmatrix} \begin{bmatrix} \underline{w_1^T} \\ \vdots \\ \vdots \end{bmatrix}$$

The first left eigen vectors of matrix  $C_{XY}C_{YX}; m \times m$

The first (largest) singular value

The square root of the largest eigenvalue of  $C_{XY}C_{YX}$  or  $C_{YX}C_{XY}$

The first right eigen vectors of matrix  $C_{YX}C_{XY}; l \times l$

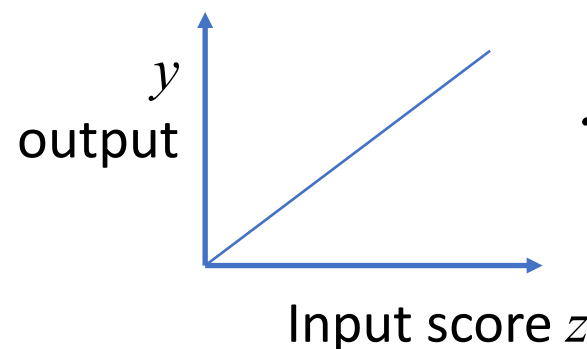
$$s_1 \geq s_2 \geq \dots$$

## Step 2. Optimal Prediction with One Latent Variable

□ In Step 1 we have found the component of the input space that is most correlated with the output;

□ We now predict output  $y$  based on the score,  $z = v^T x$

High-dimensional input vector  $x \mapsto z$  Input score: scalar  
 $z = v^T x$



Parameters to determine

$$\hat{y} = qz$$

$\hat{y} \in \mathbb{R}^{\ell \times 1}$   
 $q \in \mathbb{R}^{\ell \times 1}$

Optimal Prediction

$$\hat{y} = q^o z$$

$$q^o = \arg \min_q E[|y - \hat{y}|^2]$$

It is conceivable that this optimal coefficient/parameter vector  $q^o$  is in the same direction as unit vector  $w$ .

(This is a problem involved in the next assignment.)

Obtaining optimal  $q^0$

$$\hat{y} = qz = qv^T x$$

$$\begin{aligned} E[(y - \hat{y})^T (y - \hat{y})] &= E[(y - qv^T x)^T (y - qv^T x)] \\ &= E[y^T y - 2y^T qv^T x + x^T vq^T qv^T x] \\ &= E[y^T y - 2v^T xy^T q + v^T xx^T vq^T q] \\ &= E[y^T y] - 2v^T E[xy^T]q + v^T E[xx^T]vq^T q \end{aligned}$$

Note that  $x$  and  $y$  are random variables,  $v$  and  $q$  are not.

The necessary conditions for optimality

$$\frac{d}{dq} = 0 \quad -2 \underbrace{E[xy^T]}_{C_{YX}; \ell \times m} v + 2qv^T \underbrace{E[xx^T]}_{C_{XX}; m \times m} v = 0$$

$$\therefore q^o = \frac{C_{YX}v}{v^T C_{XX}v}$$

This is called **Output Loading Vector**.

(We omit superscript o hereafter.)

### Step 3. Deflation

- ❑ We have found just one set of latent variables associated with the highest correlation between input and output.
- ❑ But, an accurate prediction cannot be obtained with just one set of latent variables. Now we want to find the components of the second and the third highest correlation.
- ❑ The singular Value decomposition of the cross-correlation matrix, however, does not directly give the second and the third most significant latent variables.

$$C_{XY} = \begin{bmatrix} v_1 & \textcircled{v_2} & \cdots \end{bmatrix} \begin{bmatrix} s_1 & \cdots & 0 \\ \vdots & \textcircled{s_2} & 0 \\ 0 & 0 & \ddots \end{bmatrix} \begin{bmatrix} w_1^T \\ \textcircled{w_2^T} \\ \vdots \end{bmatrix}$$

These do not provide the latent variables that are second most significant (correlated).

- ❑ To overcome this difficulty, we have to go through the procedure called “Deflation”.

## Deflation

- ❑ Predicting output  $y$  based on the first set of latent variables, we have used some components involved in the data matrix;
- ❑ This component of data matrix must not be used for determining the second most significant component;
- ❑ We have to remove the components already used in the first round prediction, and examine the residual components that have the highest correlation with output.
- ❑ Output data

Original  
data

$$y' = y - (\text{the component used for the first round output prediction})$$

Residue

- ❑ Using the output loading vector  $q$ , the deflated output vector is given by

$$y' = y - zq$$

- ❑ The deflation of input data matrix is a bit more involved. Collectively, we can write

$$X' = X - (\text{components used in the 1st round})$$



# Input Data Deflation: Finding the components used in the 1<sup>st</sup> round

- ❑ The input data matrix can be written as a collection of row vectors,

$$X = \begin{pmatrix} \mathbf{x}^{(1)} & \dots & \mathbf{x}^{(N)} \end{pmatrix} = \begin{pmatrix} x_1^{(1)} & \dots & x_1^{(N)} \\ \vdots & \vdots & \vdots \\ x_m^{(1)} & \dots & x_m^{(N)} \end{pmatrix} = \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_m \end{pmatrix}$$

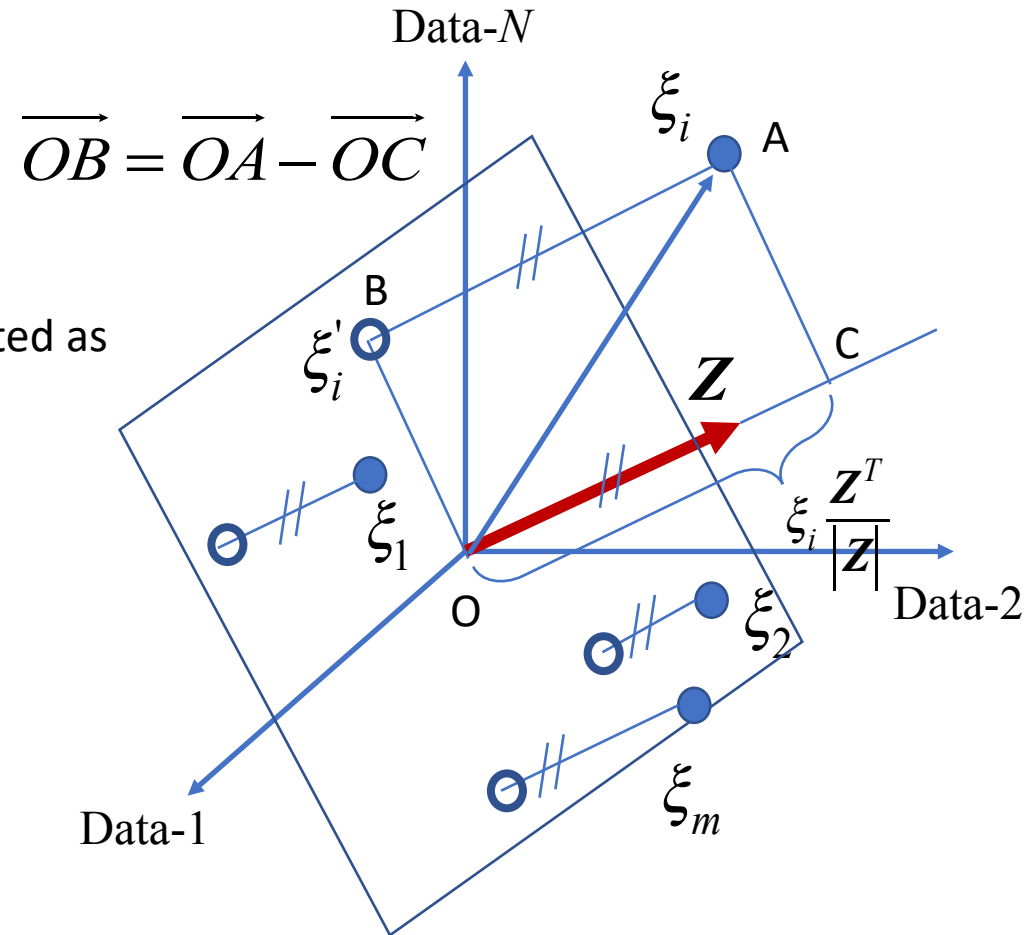
- ❑ The score of each data point from  $\mathbf{x}^{(1)}$  to  $\mathbf{x}^{(N)}$  can be collectively represented as

$$\mathbf{z} = \mathbf{v}^T \mathbf{x} \longrightarrow \begin{pmatrix} z^{(1)} & \dots & z^{(N)} \end{pmatrix} = \mathbf{Z}$$

- ❑ Plot  $\mathbf{Z}$  in  $N$ -dimensional space together with  $\xi_1, \dots, \xi_m$
- ❑ The direction of vector  $\mathbf{Z}$  indicates the distribution of scores among the  $N$  data points at which the first round latent variables have extracted information from the original data for predicting the output.
- ❑ We need to delete these components already used in the first round.
- ❑ Projecting  $\xi_i$  onto the plane perpendicular to vector  $\mathbf{Z}$  yields

$$\xi'_i = \xi_i - \underbrace{\xi_i \frac{\mathbf{Z}^T}{|\mathbf{Z}|}}_{\text{Magnitude}} \cdot \underbrace{\frac{\mathbf{Z}}{|\mathbf{Z}|}}_{\text{Direction}} = \xi_i \left( I - \frac{\mathbf{Z}^T \mathbf{Z}}{|\mathbf{Z}|^2} \right)$$

Or collectively,  $X' = X \left( I - \frac{\mathbf{Z}^T \mathbf{Z}}{|\mathbf{Z}|^2} \right)$



Note that vectors  $\mathbf{Z}$  and  $\xi_i$  are row vectors.

## Input Loading Vector

□ Let us rewrite 
$$X' = X \left( I - \frac{\mathbf{Z}^T \mathbf{Z}}{|\mathbf{Z}|^2} \right)$$

□ Note that 
$$\mathbf{Z} = \begin{pmatrix} z^{(1)} & \dots & z^{(N)} \end{pmatrix} = \begin{pmatrix} \mathbf{v}^T \mathbf{x}^{(1)} & \dots & \mathbf{v}^T \mathbf{x}^{(N)} \end{pmatrix} = \mathbf{v}^T X$$

□ Therefore 
$$|\mathbf{Z}|^2 = \mathbf{Z} \mathbf{Z}^T = \mathbf{v}^T X X^T \mathbf{v} \cong \mathbf{v}^T C_{XX} \mathbf{v}$$

□ The above deflated data matrix can be written as

$$\begin{aligned} X' &= X \left( I - \frac{\mathbf{Z}^T \mathbf{Z}}{|\mathbf{Z}|^2} \right) = X - \frac{1}{\mathbf{v}^T C_{XX} \mathbf{v}} X \mathbf{Z}^T \mathbf{Z} = X - \frac{1}{\mathbf{v}^T C_{XX} \mathbf{v}} X X^T \mathbf{v} \mathbf{v}^T X \\ &= X - \frac{1}{\mathbf{v}^T C_{XX} \mathbf{v}} C_{XX} \mathbf{v} \mathbf{v}^T X = \left( I - \frac{C_{XX} \mathbf{v} \mathbf{v}^T}{\mathbf{v}^T C_{XX} \mathbf{v}} \right) X \end{aligned}$$

□ For each column vector 
$$\mathbf{x}' = \left( I - \frac{C_{XX} \mathbf{v} \mathbf{v}^T}{\mathbf{v}^T C_{XX} \mathbf{v}} \right) \mathbf{x} = \mathbf{x} - \frac{C_{XX} \mathbf{v}}{\mathbf{v}^T C_{XX} \mathbf{v}} \mathbf{v}^T \mathbf{x} = \mathbf{x} - p \cdot \mathbf{z}$$

where 
$$p = \frac{C_{XX} \mathbf{v}}{\mathbf{v}^T C_{XX} \mathbf{v}}$$
 Is called **Input Loading Vector**.



## Properties of the Deflated Input Data Matrix and the Input Loading Vector

We can show that, with the input loading vector  $p$ , the deflated data matrix becomes the smallest.

$$\begin{aligned}
 p^o &= \arg \min_p E[|x'|^2] \quad \leftarrow x' = x - zp = x - pv^T x = (I - pv^T)x \\
 &= \arg \min_p E[x^T (I - pv^T)^T (I - pv^T)x] \\
 &= \arg \min_p \left\{ E[x^T x] - 2p^T E[xx^T]v + p^T pv^T E[xx^T]v \right\}
 \end{aligned}$$

Necessary conditions for min.

$$\frac{d}{dp} = 0 \quad 2C_{XX}v + 2pv^T C_{XX}v = 0 \quad \therefore p^o = \frac{C_{XX}v}{v^T C_{XX}v}$$

This is the same as the input loading vector. Therefore, the loading vector minimizes the deflated data matrix. In other words, the 1<sup>st</sup> round latent variables have taken the most information.

$$\text{Input Deflation} \quad x' = (I - p^o v^T)x = \left( I - \frac{C_{XX}vv^T}{v^T C_{XX}v} \right)x \quad \text{Output Deflation :} \quad y' = y - zq^o$$

Question:

Why is  $p$  not aligned with  $v$ ?

If  $C_{XX}$  is the identity matrix,  $v$  and  $p$  are aligned. However, the data are distributed not uniformly over the input space:

$$C_{XX} \neq \kappa I$$

## Deflated Covariance and Cross-Covariance Matrices $C'_{XX}$ and $C'_{YX}$

To compute the second set of latent variables, we need

$$C'_{XX} = E[x'(x')^T] \quad C'_{YX} = E[y'(x')^T]$$

for the deflated input and output data.

$$\begin{aligned} C'_{XX} &= E[(I - pv^T)xx^T(I - vp^T)] \leftarrow x' = (I - pv^T)x \\ &= (I - pv^T)E[xx^T](I - vp^T) \\ &= C_{XX} - pv^T C_{XX} - C_{XX}vp^T + pv^T C_{XX}vp^T \\ &= C_{XX} - pv^T C_{XX} \leftarrow pv^T C_{XX}v = C_{XX}v, p = \frac{C_{XX}v}{v^T C_{XX}v} \end{aligned}$$

$$C'_{XX} = (I - pv^T)C_{XX} \quad \text{Similarly, } C'_{YX} = C_{YX}(I - vp^T)$$

## Partial Least Squares Regression : Summary

The most significant  $m^*$  sets of latent variables are obtained recursively,

$$C_{XX}[1] = E[xx^T], \quad C_{YX}[1] = E[yx^T]$$

For  $k = 1$  to  $m^*$

$$C_{XX}[k+1] = (I - p[k]v^T[k])C_{XX}[k];$$

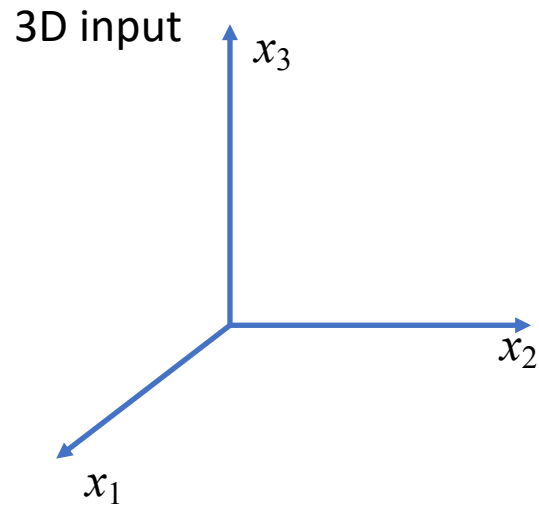
$$C_{YX}[k+1] = C_{YX}[k](I - v[k]p^T[k]);$$

$$p[k] = \frac{C_{XX}[k]v[k]}{v[k]^T C_{XX}[k]v[k]} \quad q[k] = \frac{C_{YX}[k]v[k]}{v[k]^T C_{XX}[k]v[k]}$$

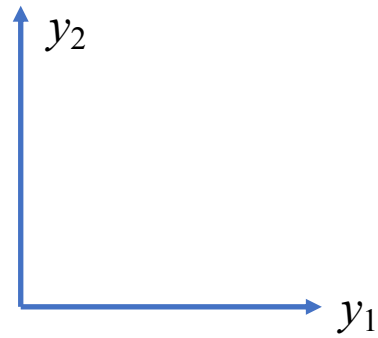
With these loading vectors,  $x$  and  $y$  can be approximated to

$$x = \sum_{k=1}^{m^*} z[k]p[k] + x[m^*] \quad y = \sum_{k=1}^{m^*} z[k]q[k] + y[m^*]$$

## Example



2D output



True relationship

$$y = Bx + g$$

$$B = \begin{pmatrix} 0.341 & 0.534 & 0.727 \\ 0.309 & 0.836 & 0.568 \end{pmatrix}$$

Input Covariance

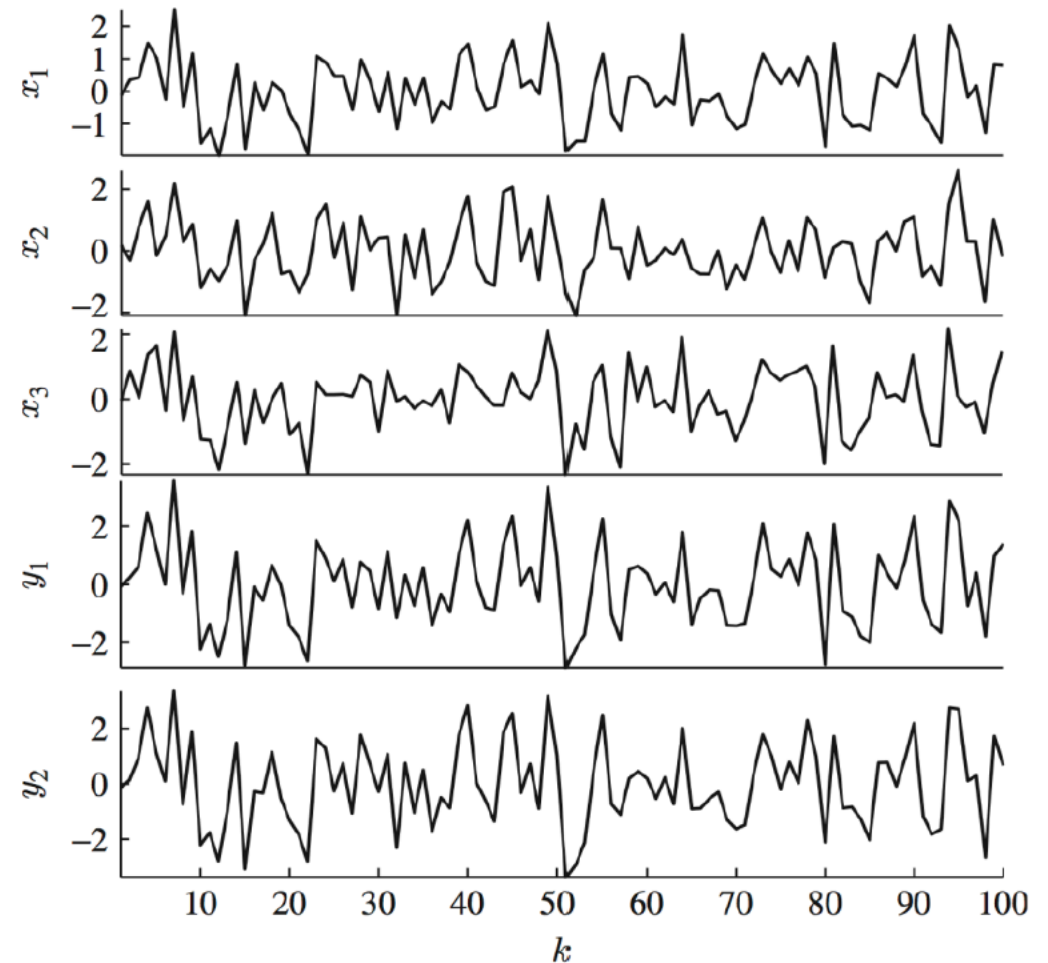
$$C_{xx} = \begin{pmatrix} 1 & 0.8 & 0.9 \\ 0.8 & 1 & 0.5 \\ 0.9 & 0.5 & 1 \end{pmatrix}$$

Input-Output Cross-Covariance

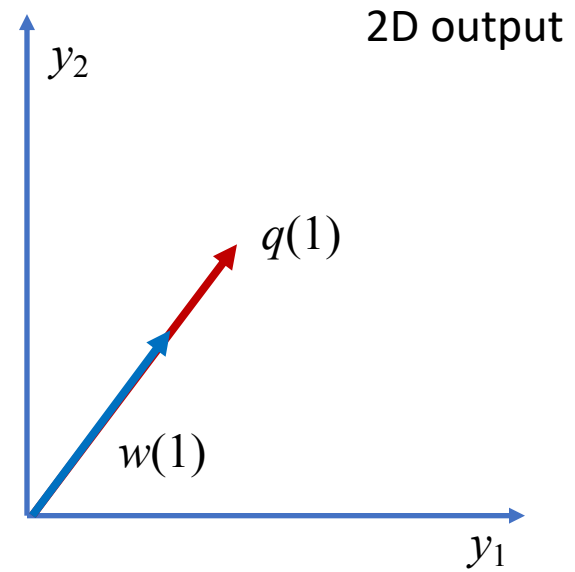
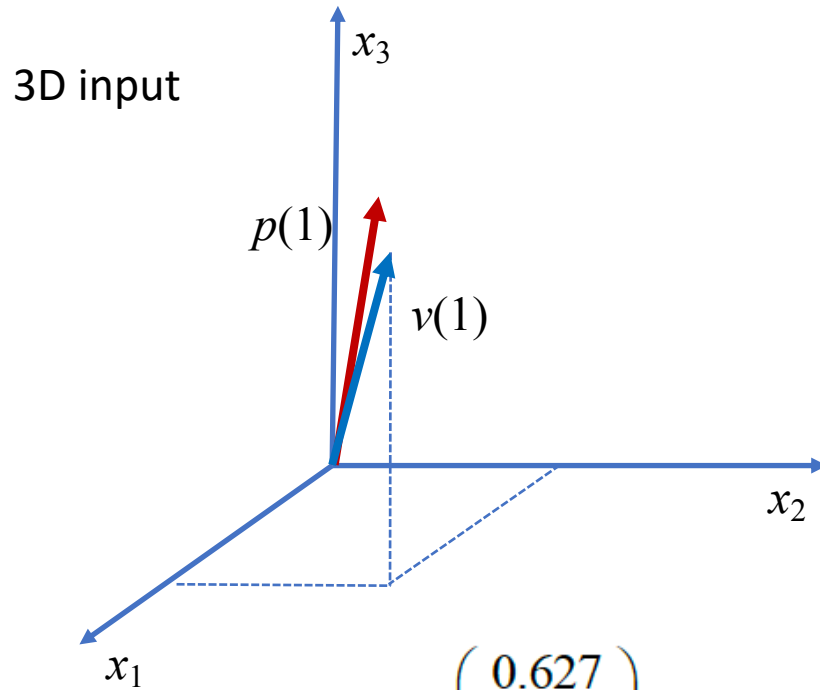
$$C_{yx} = \begin{pmatrix} 1.42 & 1.17 & 1.30 \\ 1.49 & 1.37 & 1.27 \end{pmatrix}$$

Sample Data (sample size = 100)

Data are generated with the linear model  
+ Gaussian noise  $g \sim N(0, 0.05I)$



# First Round Latent Variables



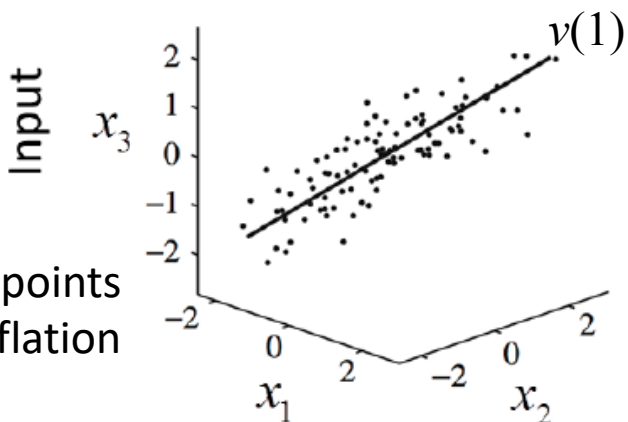
$$v(1) = \begin{pmatrix} 0.627 \\ 0.5515 \\ 0.550 \end{pmatrix}, \quad w(1) = \begin{pmatrix} 0.679 \\ 0.734 \end{pmatrix}, \quad p(1) = \begin{pmatrix} 0.631 \\ 0.536 \\ 0.561 \end{pmatrix}, \quad q(1) = \begin{pmatrix} 0.915 \\ 0.989 \end{pmatrix}$$

Singular Value Decomposition  
of the cross-correlation  
matrix

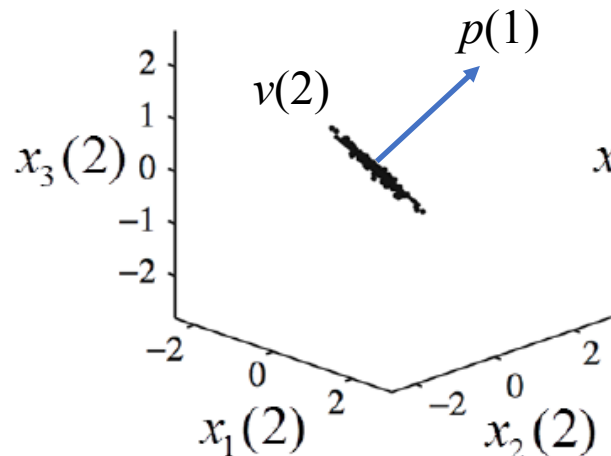
$$C_{XY} = \begin{bmatrix} v_1 & \dots \end{bmatrix} \begin{bmatrix} s_1 & \dots & 0 \\ \vdots & * & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} w_1^T \\ \vdots \\ \vdots \end{bmatrix} \quad p = \frac{C_{XX}v}{v^T C_{XX}v} \quad q = \frac{C_{YX}v}{v^T C_{XX}v}$$

# Partial Least Squares Regression

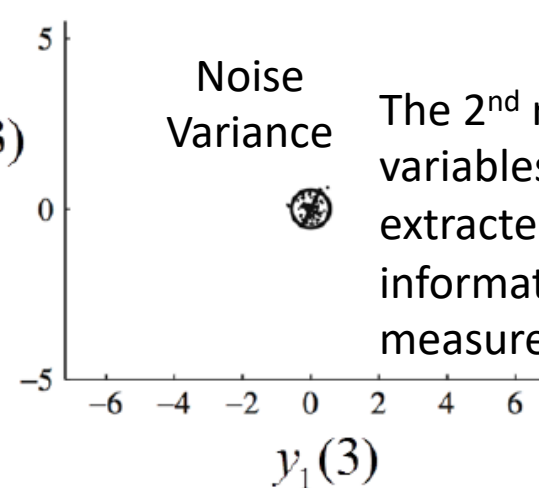
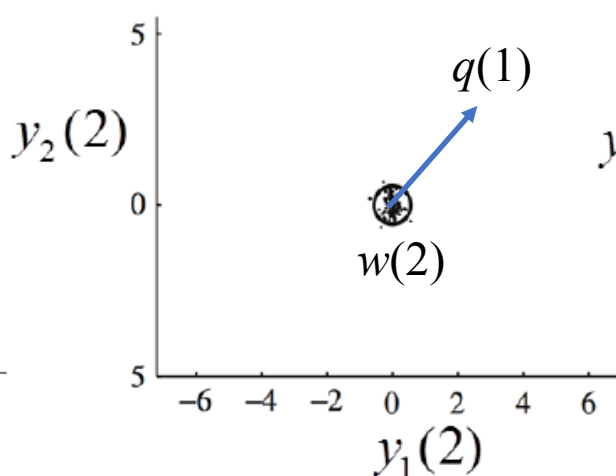
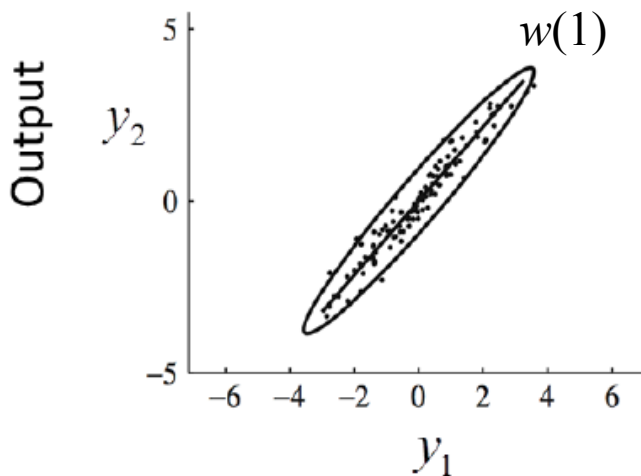
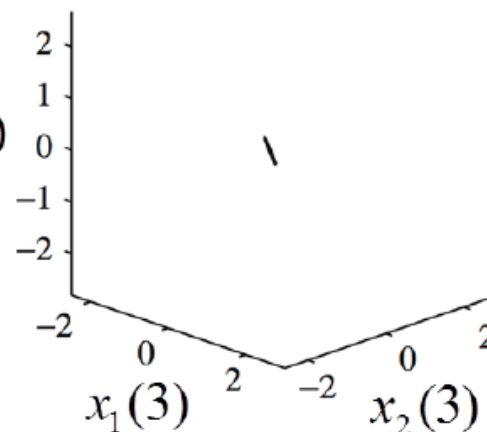
1-st round



2-nd round



3-rd round



Noise  
Variance

The 2<sup>nd</sup> round latent variables completely extracted all meaningful information, leaving only measurement noise.

The original data are deflated in the direction of  $p(1)$  for input and that of  $q(1)$  for output.

# Applications of Partial Least Squares Regression (PLSR)

☐ Chemistry

☐ Biology

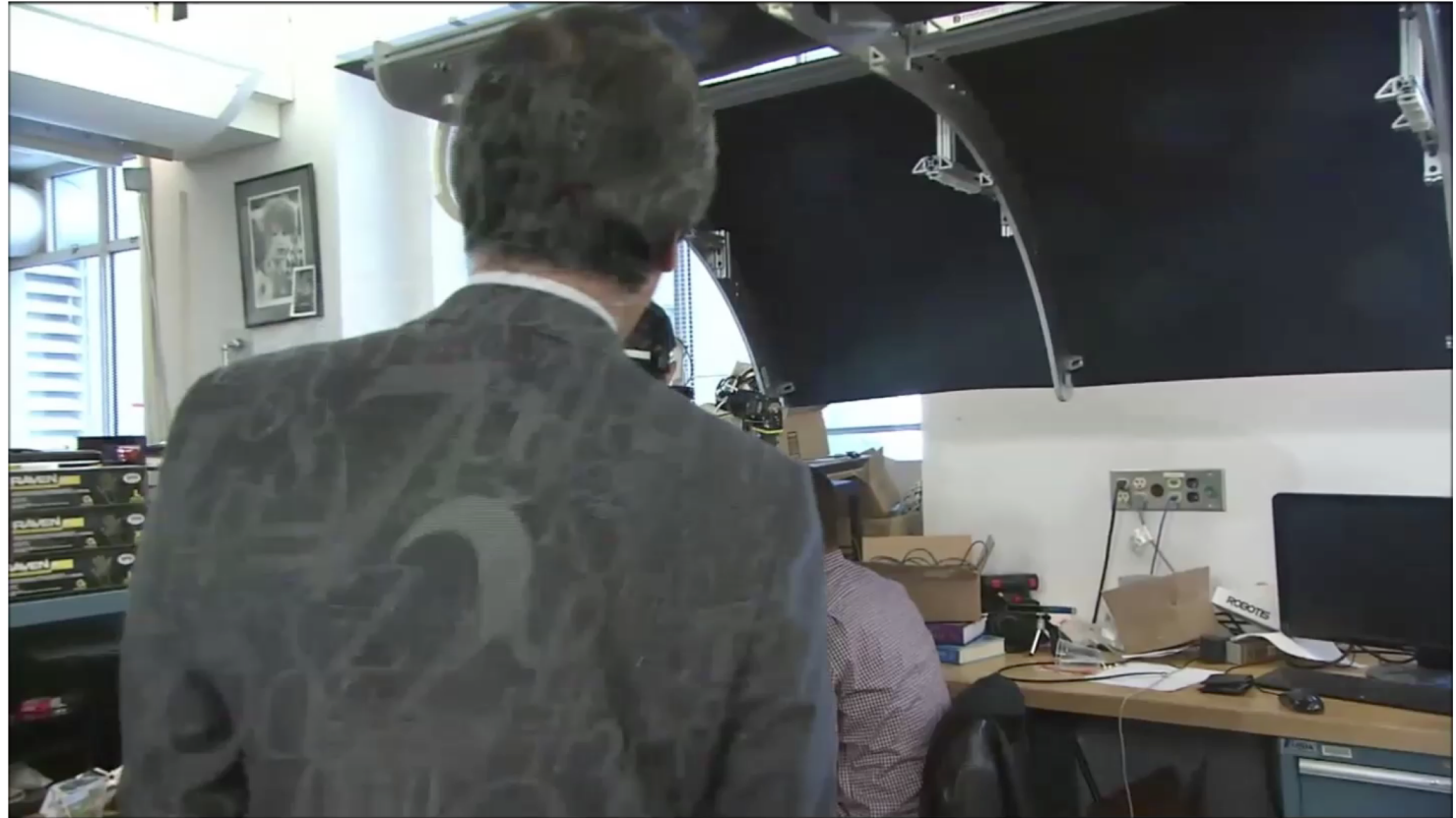
☐ Biomechanics

☐ Robotics

☐ Social Science

# Applications of Partial Least Squares Regression (PLSR)

- ☐ Chemistry
- ☐ Biology
- ☐ Biomechanics
- ☐ Robotics
- ☐ Social Science





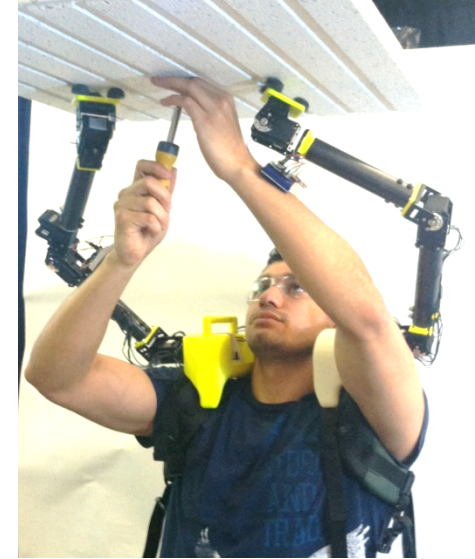
# Leader-Follower Approach

## Two-Person Demonstration



The robot arms are back-drivable.

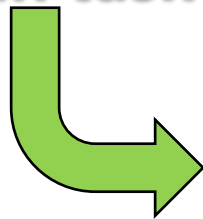
## Robot = Follower



## Human = Leader

**Observe**  
two-human task execution

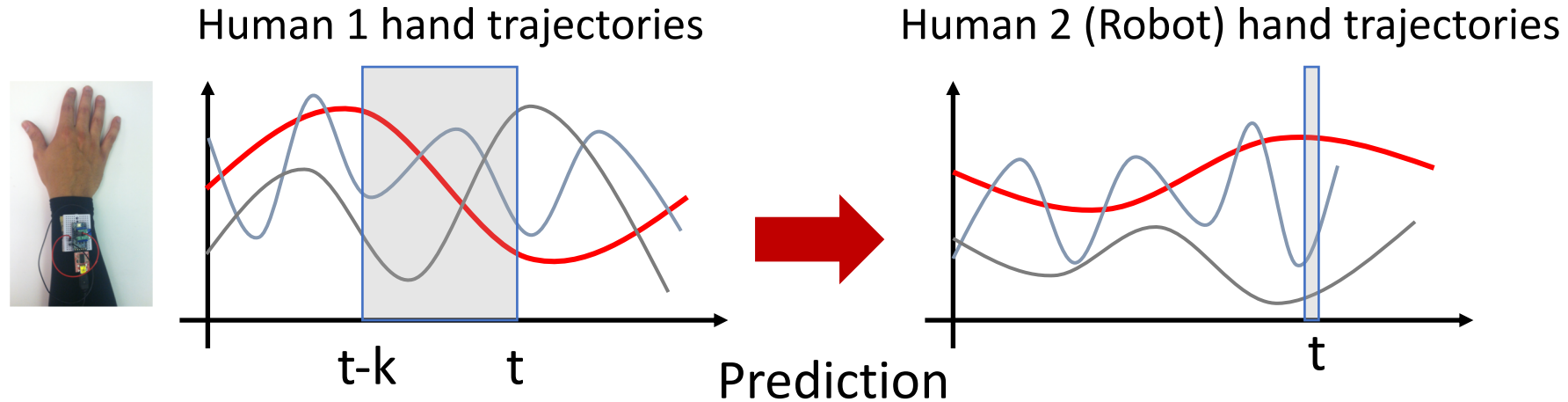
**Transfer**  
The identified laws to the robot



**Extract**  
Dynamic Coordination  
Control Laws



# Extracting Coordinated Control Laws from teaching data by using **Partial Least Squares Regression**



## Input

$\mathbf{x}$  = (3 axes of acceleration and  
3 axes of angular velocity  
of both hands at time  $\mathbf{t}$ ;  
----- at time  $\mathbf{t-1}$ ;  
-----  
----- at time  $\mathbf{t-k}$ )

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}^1 \\ \vdots \\ \mathbf{x}^N \end{pmatrix} = \begin{matrix} \text{100 x 360} \end{matrix}$$

High-dimensional input space

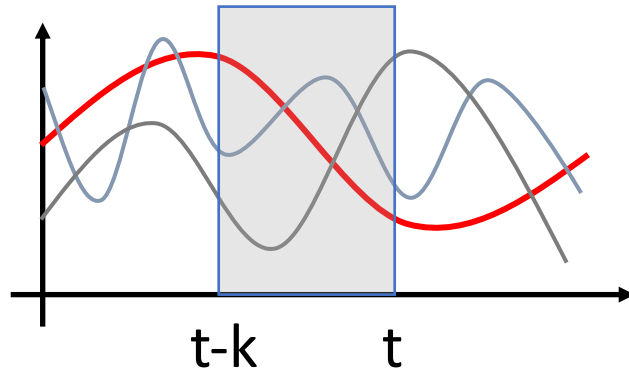
## Output

$\mathbf{y}$  = (4 joint angles of right robot arm  
4 joint angles of left robot arm at time  $\mathbf{t}$ )  
Output joint displacements may be  
collinear and correlated to each other.

$$\mathbf{Y} = \begin{pmatrix} \mathbf{y}^1 \\ \vdots \\ \mathbf{y}^N \end{pmatrix} = \begin{matrix} \text{100 x 8} \end{matrix}$$

# Four Arm Coordination

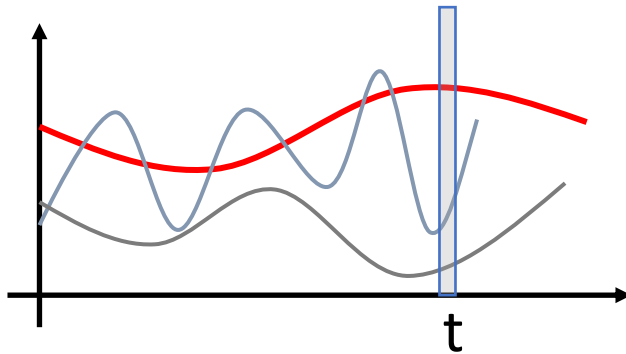
Human 1 hand trajectories



Prediction

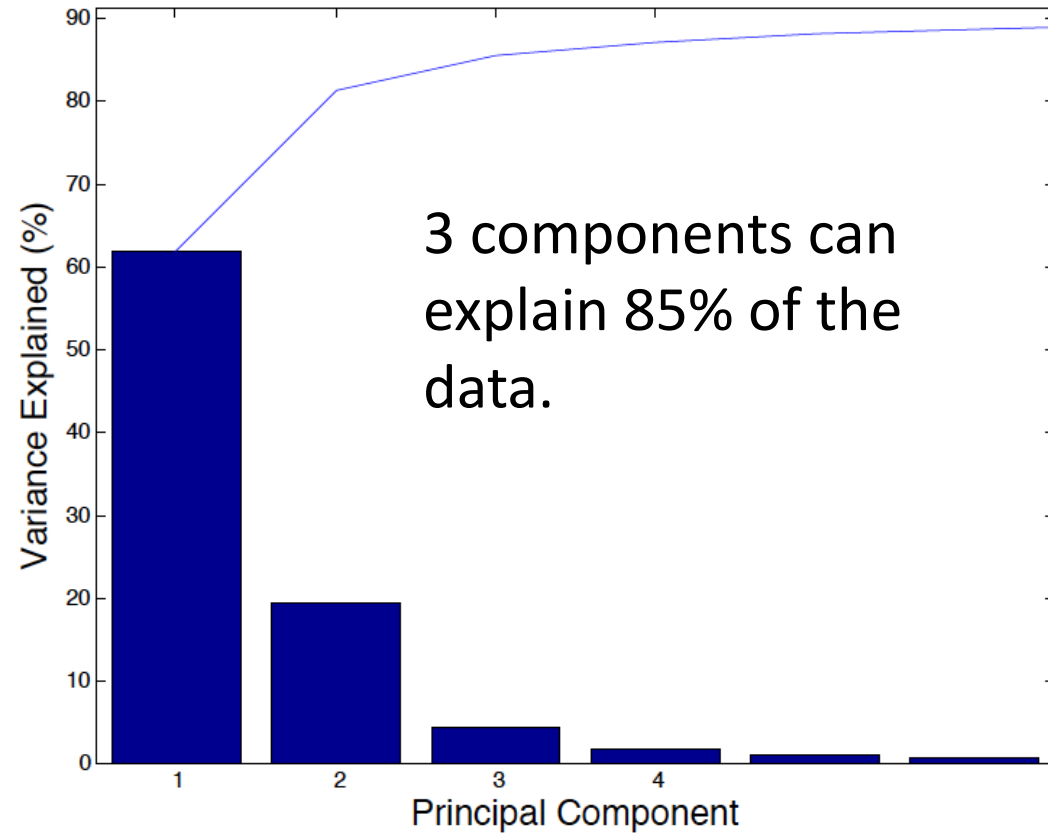


Human 2 (Robot) hand trajectories

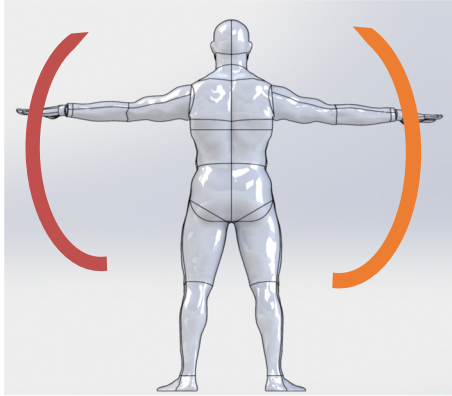


## PLS Analysis

Partial Least Squares Regression



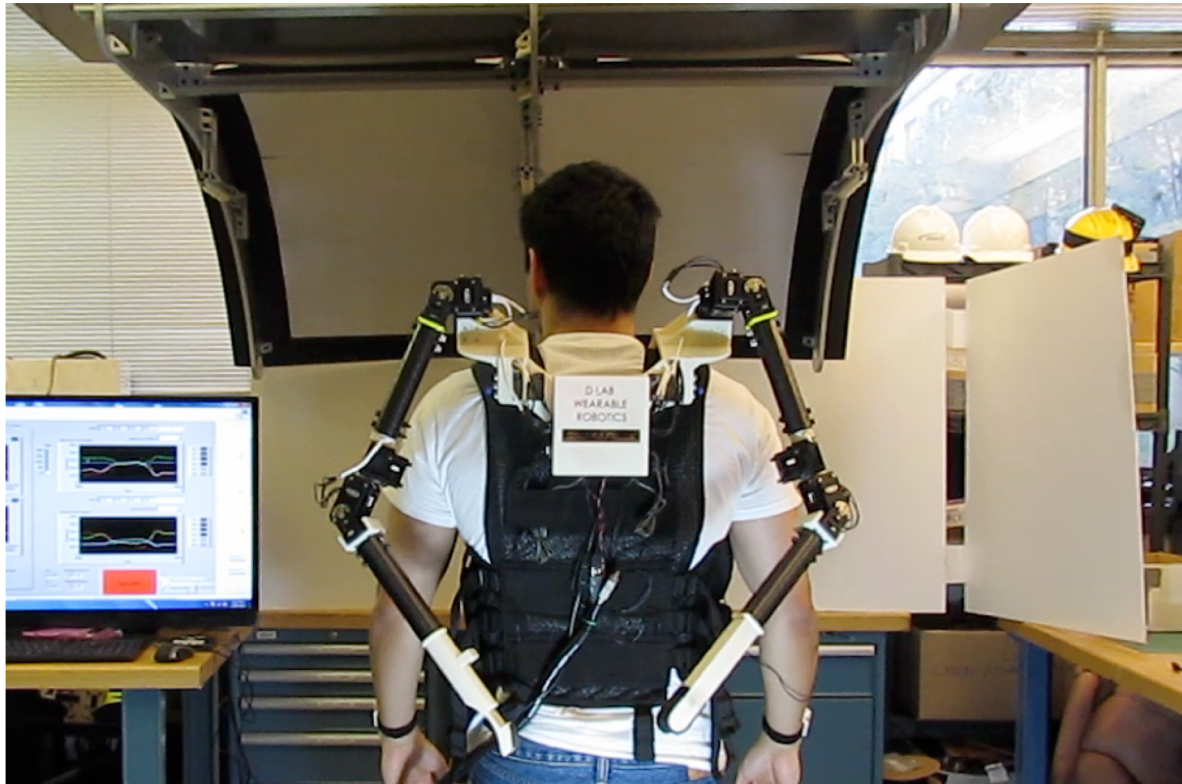
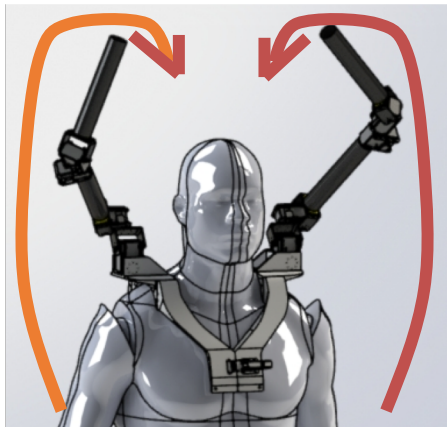
# Partial Least Squares Regression: Mode 1



Input

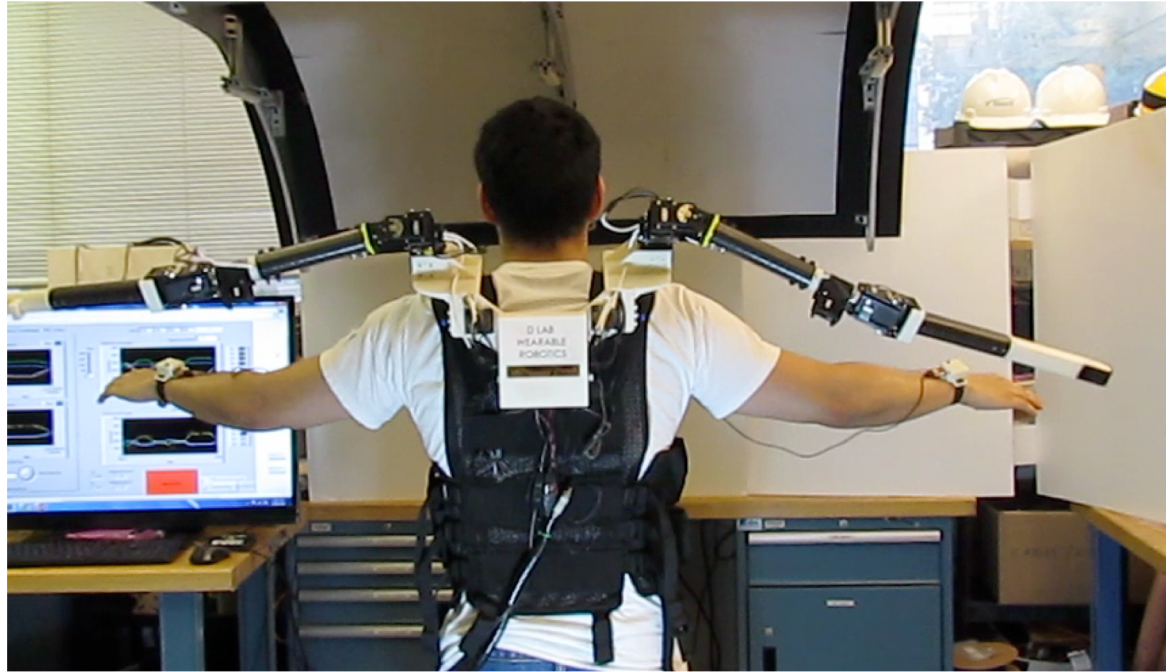
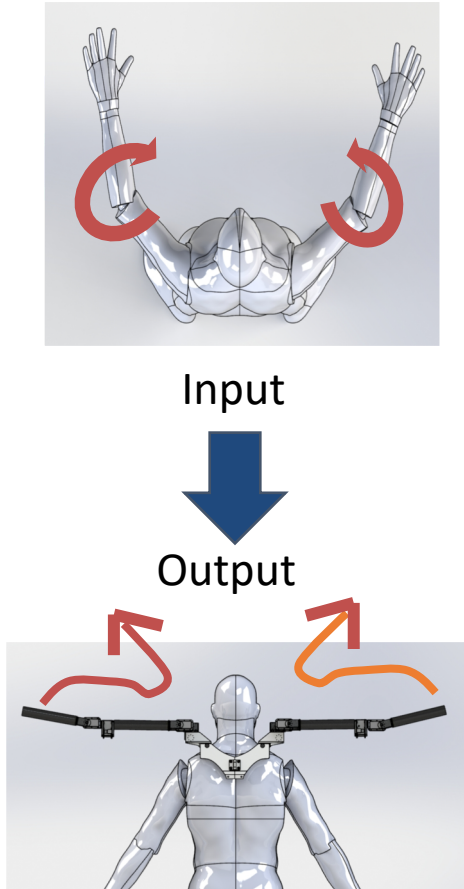


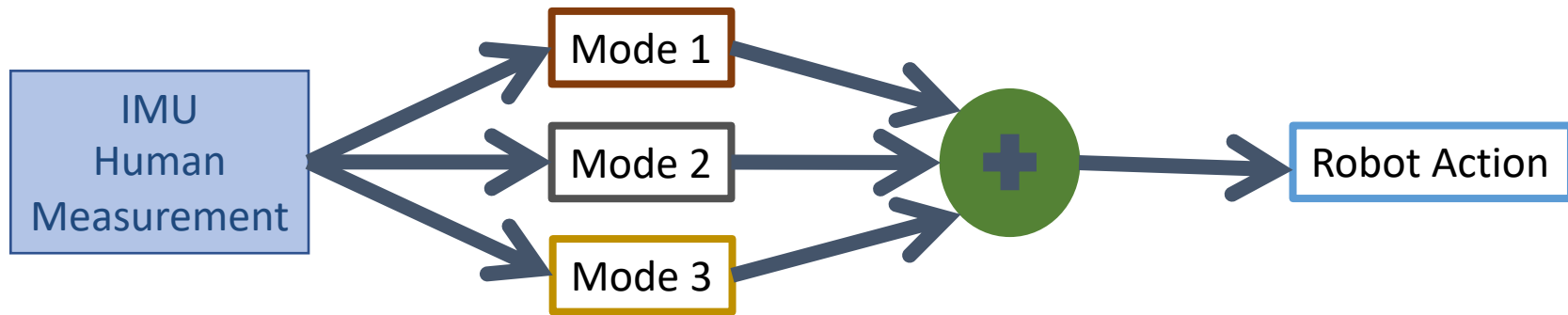
Output

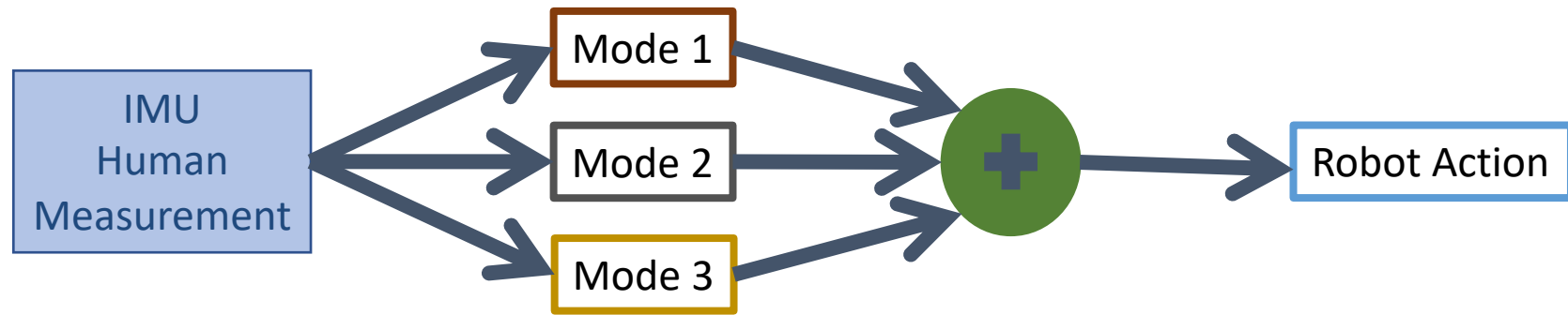




# Partial Least Squares Regression: Mode 3







# Concluding Discussion

- Dealing with high-dimensional input and output spaces is an important challenge with many practical applications of today's interest.
- PCR and PLSR are linear predictors, but as we use more input and output variables, some nonlinearities can be well captured with the high-dimensional linear regression.
- We will revisit high-dimensional spaces in Part 4. Specifically, it is closely related to extended feature space, kernel trick, and lifting linearization based on Koopman Operator and Dual-Faceted Linearization of nonlinear dynamical systems.