Principal Component Regression and Partial Least Squares

UBCO MDS — DATA 572

Motivation

- Recall: PCA is an unsupervised technique. If you look back, there is no inherent response variable (Y) that we are optimizing.
- We simply rotated our original predictors in a 'clever' manner, and toss out the rotations that do not appear to contain important information.
- We then discussed some interpretations of these rotations, etc. Rarely would this be the end of the story...

Motivation

- PCA (once you've removed some components) is generally viewed as a dimensionality reduction technique.
- Most commonly, you'll be interested in taking that reduced space, and using it for more machine learning! (Be it supervised, or unsupervised)
- Let's get into some details...we'll start with the simplest setup...

Principal Components Regression

- Principal Components Regression, or PCReg for short, is the most natural (though not necessarily the most useful) form for making use of PCA in a supervised context.

- Suppose we perform PCA on X, which is an $n \times p$ matrix of observations (on p predictors), and decide to retain h components. AKA

$$\Sigma \approx \mathrm{P}\Lambda\mathrm{P}'$$

where Σ is a $p \times p$ covariance/correlation matrix, P is a $p \times h$ matrix of eigenvectors (loadings) and Λ is a $h \times h$ diagonal matrix with the h largest eigenvalues.

- We then map our $n \times p$ matrix X to an $n \times h$ matrix S via $\mathrm{S} = \mathrm{XP}$, these are the scores.

Principal Components Regression

- Suppose that a continuous response variable Y is on hand, then we can easily assume the following model for linear regression

$$Y = \beta_0 + \beta_1 S_1 + \beta_2 S_2 + \cdots + \beta_h S_h + \epsilon$$

with all the usual linear regression assumptions (for inferential purposes).

- And that's it! That is PCReg: using your retained principal components as predictors for a continuous response.

- So for practical purposes, it's straightforward. It's worth thinking a tad more deeply about what's being achieved though...

PCReg Deeper

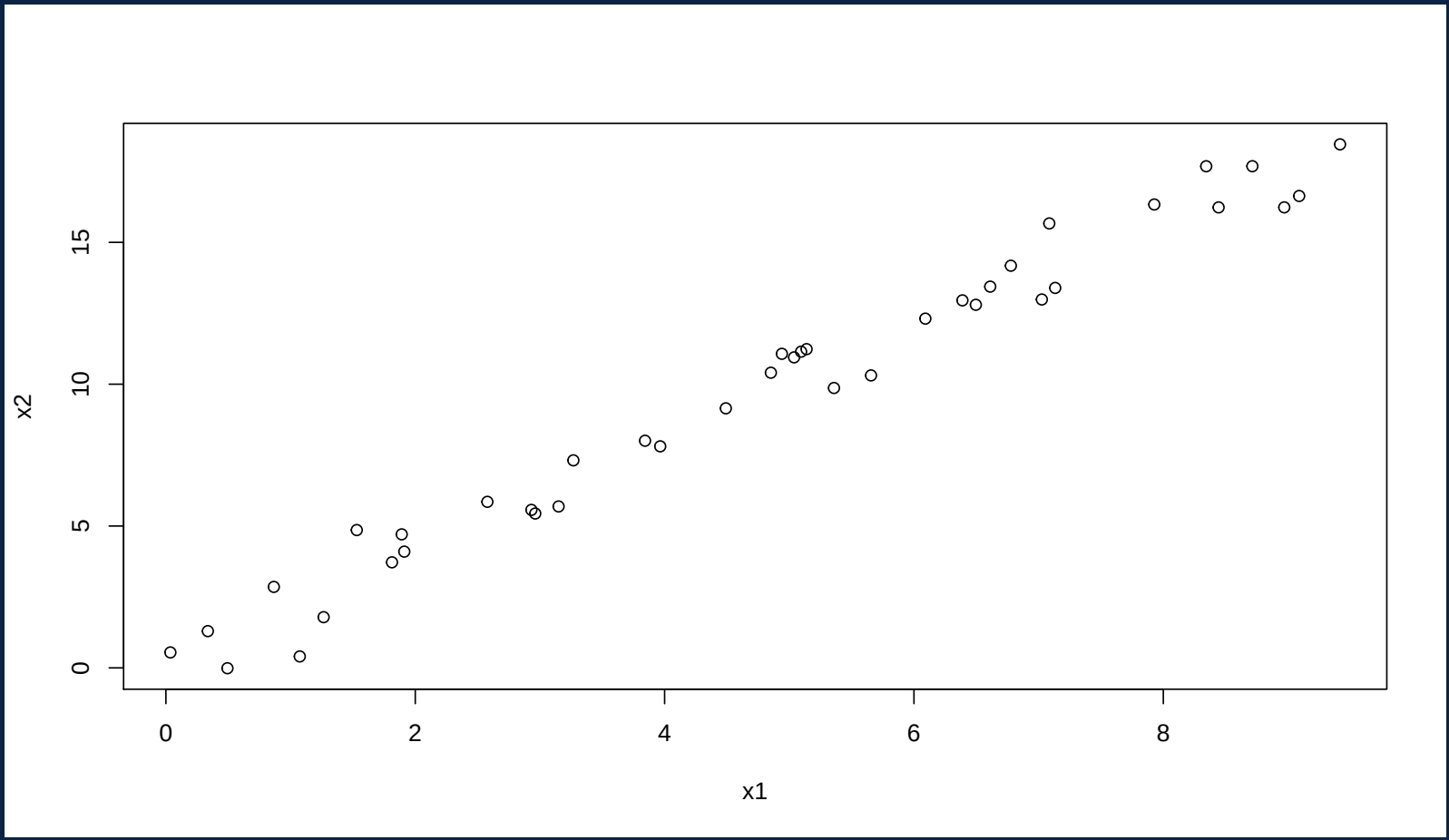
- Firstly, if $h = p$ (aka, you retain all PCs), then the model is equivalent to ordinary least squares modelling in terms of $\hat{Y}$. Obviously the estimated coefficients differ, etc...but you do not lose any predictive power as you are not losing any information.
- Next, consider a pro...
- Congratulations, you've just taken care of the problem of multicollinearity. How?

PCReg Deeper

- Finally, some cons...
- PCReg can be viewed as a discretized regularizer, removing low variance components (but not entire predictors). So it has some commonality with ridge regression, but due to ridge regression's smooth regularization, ridgereg is often a better option than PCReg.
- There is absolutely NO guarantee that higher variance components — which is with respect to the predictor space — contain more predictive power towards Y!

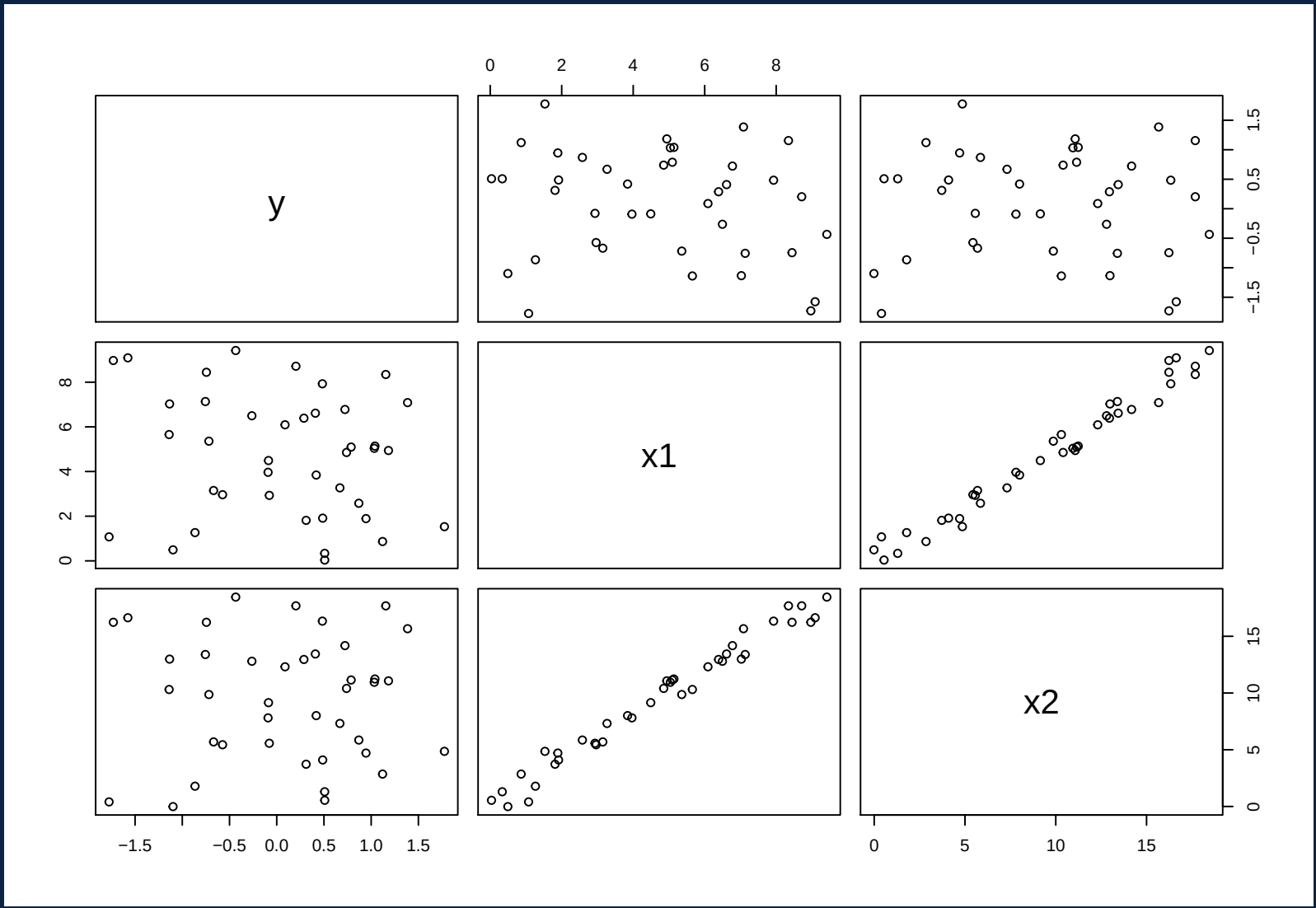
A cautionary tale...

- Recall our motivating simulation from the PCA lecture



A cautionary tale...

- I've added a response variable



A cautionary tale...

```
> linmod <- lm(y~x1+x2)
> summary(linmod)

Call:
lm(formula = y ~ x1 + x2)

Residuals:
     Min       1Q   Median       3Q      Max
-0.26489 -0.07545 -0.01078  0.08809  0.21513

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.007547   0.038730   0.195    0.847
x1          -2.040311   0.043519 -46.883   <2e-16 ***
x2           1.020113   0.022127  46.103   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.1199 on 37 degrees of freedom
Multiple R-squared:  0.9835,Adjusted R-squared:  0.9826
F-statistic:  1100 on 2 and 37 DF,  p-value: < 2.2e-16
```

A cautionary tale...

```
> pcs <- prcomp(cbind(x1, x2))
> summary(pcs)
Importance of components:
                          PC1     PC2
Standard deviation     6.0766 0.39399
Proportion of Variance 0.9958 0.00419
Cumulative Proportion  0.9958 1.00000
```

A cautionary tale...

```
> linpc <- lm(y~pcs$x[,1])
> summary(linpc)

Call:
lm(formula = y ~ pcs$x[, 1])

Residuals:
    Min      1Q  Median      3Q     Max
-1.9419 -0.7712  0.2144  0.6891  1.6439

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.08484    0.14517   0.584    0.562
pcs$x[, 1]   0.00834    0.02419   0.345    0.732

Residual standard error: 0.9181 on 38 degrees of freedom
Multiple R-squared:  0.003117,Adjusted R-squared:  -0.02312
F-statistic: 0.1188 on 1 and 38 DF,  p-value: 0.7322
```

A cautionary tale...

```
> linpc2 <- lm(y~pcs$x[,2])
> summary(linpc2)

Call:
lm(formula = y ~ pcs$x[, 2])

Residuals:
      Min        1Q    Median        3Q       Max
-0.261207 -0.080209 -0.007321  0.081190  0.261425

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.08484    0.02039   4.161 0.000174 ***
pcs$x[, 2]   2.28110    0.05241  43.527  < 2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.1289 on 38 degrees of freedom
Multiple R-squared:  0.9803,Adjusted R-squared:  0.9798
F-statistic:  1895 on 1 and 38 DF,  p-value: < 2.2e-16
```

A cautionary tale...

"But you didn't standardize!" ... okay then ...

```
> pcss <- prcomp(cbind(x1, x2), scale.=TRUE)
> summary(pcss)
Importance of components:
                          PC1     PC2
Standard deviation     1.4097 0.11337
Proportion of Variance 0.9936 0.00643
Cumulative Proportion  0.9936 1.00000
```

A cautionary tale...

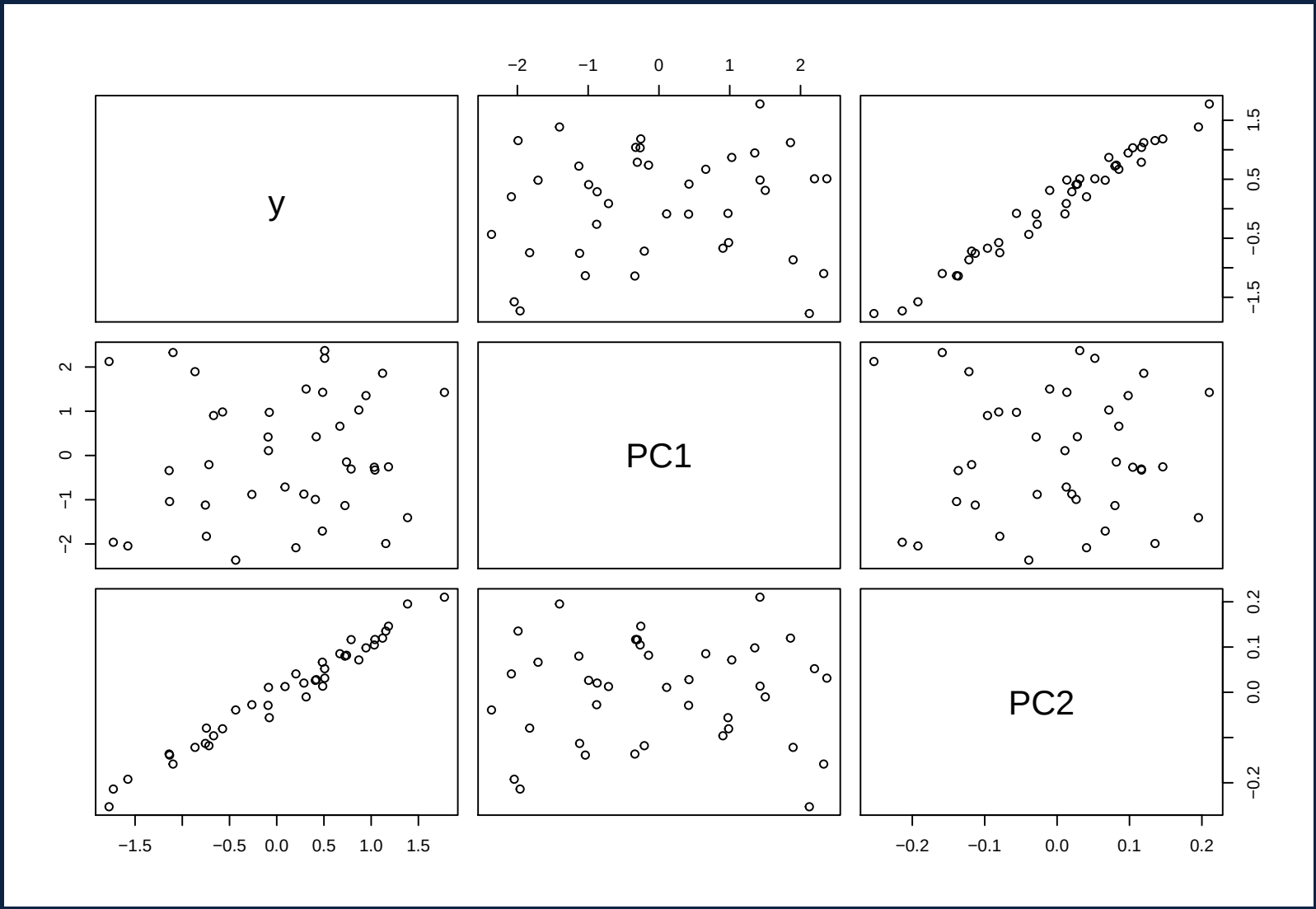
```
> linpcs <- lm(y~pcss$x[,1])
> summary(linpcs)

Call:
lm(formula = y ~ pcss$x[, 1])

Residuals:
    Min      1Q  Median      3Q     Max
-2.0009 -0.7343  0.2586  0.7136  1.5962

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.08484    0.14463   0.587    0.561
pcss$x[, 1]  0.06621    0.10390   0.637    0.528

Residual standard error: 0.9147 on 38 degrees of freedom
Multiple R-squared:  0.01057,Adjusted R-squared:  -0.01546
F-statistic: 0.4061 on 1 and 38 DF,  p-value: 0.5278
```

A cautionary tale...

```
> linpcs2 <- lm(y~pcss$x[,2])
> summary(linpcs2)

Call:
lm(formula = y ~ pcss$x[, 2])

Residuals:
      Min        1Q    Median        3Q       Max
-0.257674 -0.126315  0.009366  0.095724  0.306733

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  0.08484    0.02394   3.543  0.00107 **
pcss$x[, 2]  7.89705    0.21389  36.921  < 2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 0.1514 on 38 degrees of freedom
Multiple R-squared:  0.9729,Adjusted R-squared:  0.9722
F-statistic:  1363 on 1 and 38 DF,  p-value: < 2.2e-16
```

A cautionary tale...

- Here's the visual...



Comments

- Clearly PCReg has some issues that need fixing...
- One simple approach is to disregard the standard PCA approaches for tossing out components, and instead take all p components, then perform standard stepwise regression procedures.
- This would fix the issue with our simulation, but would not cover all potential issues.
- Leaving the problems aside for a moment, note that of course PCs can be used as predictors in any supervised context (random forests, neural nets, discriminant analysis, etc).

Partial Least Squares

- A more proper approach is to somehow consider the response variable Y while performing the PCA in the first place!
- Partial Least Squares (PLS) does exactly this.
- It seeks linear combos of predictors that have high variance AND high correlation with Y .
- Just like PCA, it is not scale invariant. Therefore, the predictors are generally scaled to have mean 0 variance 1.

PLS Algorithm

Algorithm 3.3 *Partial Least Squares.*

1. Standardize each $\mathbf{x}_j$ to have mean zero and variance one. Set $\hat{\mathbf{y}}^{(0)} = \bar{y}\mathbf{1}$, and $\mathbf{x}_j^{(0)} = \mathbf{x}_j,\ j = 1, \ldots, p$.
2. For $m = 1, 2, \ldots, p$
   (a) $\mathbf{z}_m = \sum_{j=1}^{p} \hat{\varphi}_{mj}\mathbf{x}_j^{(m-1)}$, where $\hat{\varphi}_{mj} = \langle \mathbf{x}_j^{(m-1)}, \mathbf{y} \rangle$.
   (b) $\hat{\theta}_m = \langle \mathbf{z}_m, \mathbf{y} \rangle / \langle \mathbf{z}_m, \mathbf{z}_m \rangle$.
   (c) $\hat{\mathbf{y}}^{(m)} = \hat{\mathbf{y}}^{(m-1)} + \hat{\theta}_m \mathbf{z}_m$.
   (d) Orthogonalize each $\mathbf{x}_j^{(m-1)}$ with respect to $\mathbf{z}_m$: $\mathbf{x}_j^{(m)} = \mathbf{x}_j^{(m-1)} - [\langle \mathbf{z}_m, \mathbf{x}_j^{(m-1)} \rangle / \langle \mathbf{z}_m, \mathbf{z}_m \rangle]\mathbf{z}_m,\ j = 1, 2, \ldots, p$.
3. Output the sequence of fitted vectors $\{\hat{\mathbf{y}}^{(m)}\}_1^p$. Since the $\{\mathbf{z}_\ell\}_1^m$ are linear in the original $\mathbf{x}_j$, so is $\hat{\mathbf{y}}^{(m)} = \mathbf{X}\hat{\beta}^{\text{pls}}(m)$. These linear coefficients can be recovered from the sequence of PLS transformations.

From Elements of Statistical Learning. This is the classical algorithm, others have been put forth.

A cautionary tale...

```
> plsmod <- plsr(y~x1+x2, method="oscorespls")
> summary(plsmod)
Data:  X dimension: 40 2
Y dimension: 40 1
Fit method: oscorespls
Number of components considered: 2
TRAINING: % variance explained
   1 comps  2 comps
X   99.033   100.00
y    1.672    98.35
```

Note that the extremely high variance that I manufactured within the predictors still drives the first component. However, the output at least makes this clear to us!

PLS Comments

- There are PLS versions for classification tasks as well (PLS-DA for example), and plenty of extensions/refinement.
- PLS originated in the 80's after all.
- It is the predominant model in several applied fields (some chemistry fields, sensory sciences, marketing, and more).
- This is likely due to its inherent interpretability (linear combos), in addition to being an early solution to the problem of moderate-to-high dimensionality.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