A Comparison on multi-response multivariate estimation methods

Raju Rimal, Trygve Almøy and Solve Sæbø 03 Apr, 2018

Contents

1	Introduction	1
	1.1 Background	1
	1.2 Objective	1
2	Statistical Model	2
3	Exerimental Design	2
4	Estimation Methods	2
5	Exploratory Study	3
6	Systematic Comparison	3
7	Discussion and Conclusion	4

1 Introduction

- "Big Data" is becoming a focal discussion in most of the discipline
- Massive explosion of data with informations integrated in many variables and features
- New methods and algoriths are being devised inorder to extract such information and study the relationship between different variables
- Modern inter-disciplinary research fields such as chemometrics, echonometrics and bioinformatics are handling multi-response models extensively
- This paper attempts to compare some of such methods and their performance on linear model data with specifically designed properties

1.1 Background

- Discuss some previous study on comparison specifically on multi-response setting
- Discuss the experimenal design settings on those papers
- What is new thing about this paper that other have not done

1.2 Objective

- Demonstrate a systematic comparison study using SimrelM
- Compare new estimation methods with conventional methods using data with properties particularly constructed for comparison

2 Statistical Model

Simulation model

$$\begin{bmatrix} \mathbf{y} \\ \mathbf{x} \end{bmatrix} \sim \mathbf{N} \left(\begin{bmatrix} \boldsymbol{\mu}_y \\ \boldsymbol{\mu}_x \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{yy} & \boldsymbol{\Sigma}_{yx} \\ \boldsymbol{\Sigma}_{xy} & \boldsymbol{\Sigma}_{xx} \end{bmatrix} \right)$$

- Define transformation as z = Rx and w = Qy
- Equivalent latent model will be,

$$\begin{bmatrix} \mathbf{w} \\ \mathbf{z} \end{bmatrix} \sim \mathbf{N} \left(\begin{bmatrix} \boldsymbol{\mu}_w \\ \boldsymbol{\mu}_x \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{ww} & \boldsymbol{\Sigma}_{wz} \\ \boldsymbol{\Sigma}_{zw} & \boldsymbol{\Sigma}_{zz} \end{bmatrix} \right)$$

• How much should I discuss about simrel-M??

3 Exerimental Design

- Parameters with single level:
 - Number of observations (n): 100
 - Number of response variables (m): 3
 - Number of informative response components: 2
 - Position of predictor components relevant for response components (relpos): 1, 4; 2, 3
 - Something smart (ypos): 1; 2, 3
- Parameters with multiple level:
 - Number of predictor variables (p): 2 levels
 - Decay factor of eigenvalues corresponding to predictors (gamma): 2 levels
 - Decay factor of eigenvalues corresponding to response (eta): 2 levels
 - Coefficient of determination corresponding to each informative response compnentsR2: 2 levels

4 Estimation Methods

- Methods used in the study and their short description (how they estimate, what are they based on)
 - 1. Principal Component Regression (PCR)
 - 2. Partial Least Squares 1 (PLS1)
 - 3. Partial Least Squares 2 (PLS2)
 - 4. Cannonical Partial Least Squares (CPLS)
 - 5. Cannonically Powered Partial Least Squares (CPPLS)
 - 6. Envelope Estimation in Predictor Space (Xenv)
 - 7. Envelope Estimation in Response Space (Yenv)
 - 8. Simulteneous envelope estimaion (Senv)
 - 9. Ridge Regression (Ridge)
 - 10. Lasso Regression (Lasso)
- How details should I discuss about these methods in terms their way of estimation and difference between them
- As *Xenv*, *Yenv* and *Senv* are based on maximum likelihood estimation, principal components of predictors explaining 99.5% of their variation are used.

5 Exploratory Study

- This section explores the inter-connection between the estimation methods and the properties of data based on regression coefficients
- Our discussion revolve around following factors and their interaction
 - Wide vs Tall predictor matrix
 - High vs Low multicollinearity
 - High vs Low correlation between responses
 - Hight vs Low coefficient of determination

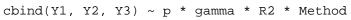
6 Systematic Comparison

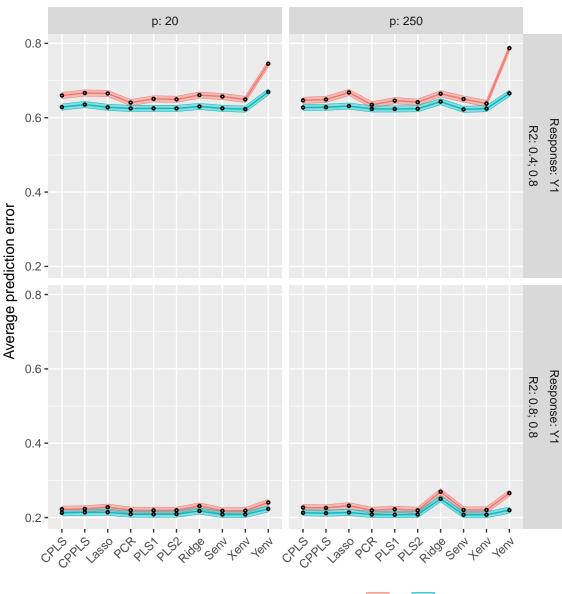
- Should we use MANOVA model or some kind of norm/trace or similar measure for the error and use ANVOA instead?
- A MANOVA model is used for statistical analysis

$$\mathtt{pred_err}_{ijkl} = \mu + \mathtt{p}_i * \mathtt{gamma}_j * \mathtt{r2}_k * \mathtt{method}_l + \epsilon_{ijkl}$$

- In the model the prediction error for each of three response variables are used as response variable and following variables (with levels) and their complete interactions are used as predictor variables.
 - a) Number of predictor variables (p): 20 and 100
 - b) Decay factor of eigenvalues of $X(\gamma)$: 0.2 and 0.8
 - c) Decay factor of eigenvalues of $Y(\eta)$: 0.1 and 0.6
 - d) Coefficient of Determination (ρ): 0.4, 0.4 and 0.4, 0.8
 - e) Method of estimation: PCR, PLS1, PLS2, CPLS, CPPLS, Xenvelope, Yenvelope, Senvelope, Ridge and Lasso
 - f) Number of tuning Parameters used (as numeric)
- An effect plot for fitted MANOVA model,

Effect plot of model:





Decay of predictor variables (gamma) - 0.2 - 0.9

7 Discussion and Conclusion