A comparetive study on PCR, PLS, Envelope and BayesPLS models

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4 September 2016

Overview

- Background
- Estimation methods under comparison
- Data Simulation
- Analysis, Results and Discussions

Background

- PLS **Population Model** [Helland, 1990] which further discussed by [Naes and Helland, 1993, Helland, 2001]
- PLS, *heavely developed* [Wold, 1985, Naes and Helland, 1993, De Jong, 1993], without addressing the population model [Cook et al., 2013]
- Mostly popular among chemometrician
- Was not very popular among statistician which has changed and is nowadays considered as an essential tool for multivariate analysis
- Accounting the population model, new estimation methods have been purposed such as **Envelope** [Cook et al., 2010, Cook and Zhang, 2016] and **BayesPLS** [Helland et al., 2012] which are *closely related* to PLS
- Cook et al. [2013] said that PLS is fundamentally an envelope in the population model

Background

- This study attempts to make an *emperial comparison* among PCR, PLS, Envelope and BayesPLS model on the basis of their **prediction ability**
- Using `simrel` [Sæbø et al., 2015] R-package, data with diverse nature are simulated.
- `simrel` allows to have control over latent structure (relevant component) of the data, fine analysis of strength and weakness of a models is possible

Statistical Model

The common ground of all the methods is to best describe (fit) the multivariate linear model below,

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon} \tag{1}$$

where,

$\boldsymbol{y}$	:	Response
$\boldsymbol{X}$	:	Matrix of p predictor variable
$\boldsymbol{\beta}$	:	Regression Coefficients
$\boldsymbol{\epsilon}$	:	Error $\epsilon \sim \text{NID}(0, \sigma^1)$

Here, both $\boldsymbol{y}$ and $\boldsymbol{X}$ are considered to be centered.

Statistical Model

All the models under this study consider a **subspace of predictor variables that is relevant for response**. They differ in the ways of finding the subspace and corresponding model estimates. The true estimates can also be written as,

$$\boldsymbol{\beta} = \Sigma_{XX}^{-1}\sigma_{Xy} = \sum_{j=1}^{p}\frac{1}{\alpha_j}\boldsymbol{e}_j\boldsymbol{e}_j^t\sigma_{Xy} = \sum_{j=1}^{p}\gamma_j\boldsymbol{e}_j$$

where,

γ_j	:	$\frac{\boldsymbol{e}_j^t\sigma_{Xy}}{\lambda_j}$
$\boldsymbol{e}_j$	:	Eigenvector of Σ_{xx}
λ_j	:	Eigenvalue of Σ_{xx}
σ_{Xy}	:	Covariance between y and X

So, True regression estimates are the space spanned by the eigenvectors of population covariance matrix Σ_{xx}.

Comparison of Methods

PCR	PLS
* Regression of response on latent space of predictor * No strict assumption	* Estimation through Iterative algorithm * No strict assumption

Envelope (MLE)	Bayes
* Estimation using Maximum Likelihood	* Estimation through MCMC approach with rotation of relevant space
* Can not be used when predictor is larger than observations	* Heavy Computation when p is large

Data Simulation

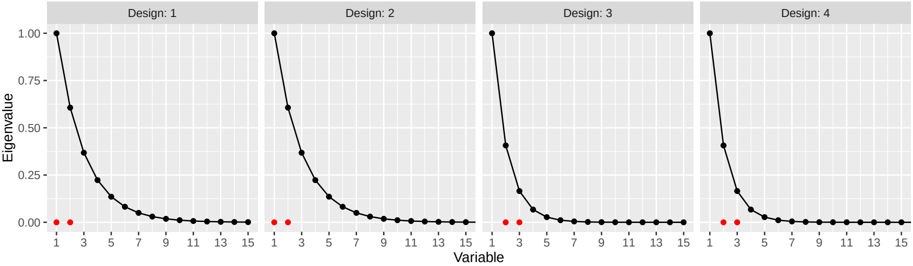
Models are analysed under diverse nature of data. Data are simulated using `simrel` package (R). In this study, I have included following four design;

n	p	R2	relpos	gamma
50	15	0.5	1, 2	0.5
50	40	0.5	1, 2	0.5
50	15	0.9	2, 3	0.9
50	40	0.9	2, 3	0.9

`n`	:	Number of observations
`p`	:	Number of variables
`R2`	:	Variation explained by the model
`relpos`	:	Position of relevant components
`gamma`	:	Reduction factor of eigenvalue of X

For each of these design, 5000 test samples are simulated.

Relevant Position and Eigenvalues

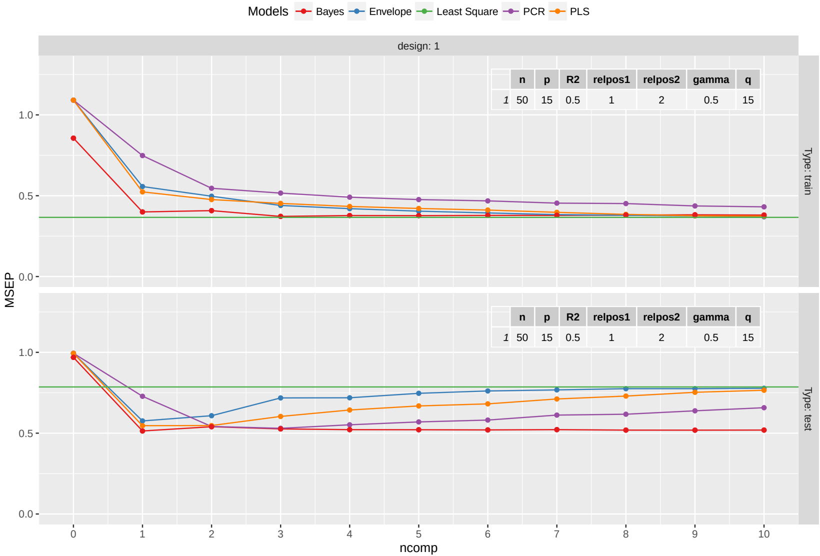


- When Relevant components are at the position of high eigenvalues, the situation is easier to model
- When Relevant components are at the position of low eigenvalues, for example 5, 10, then the most variation present in X are not relevant for Y and this will become a very difficult situation.

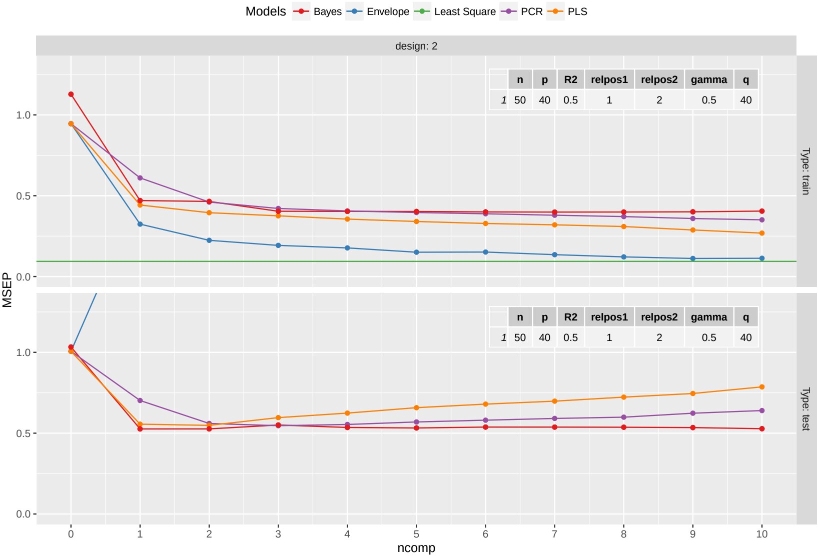
Models are compared on the basis of their prediction ability by measuring *test* and *training* **Mean Square Error of Prediction (*MSEP*)**. Mean prediction error is calculated as,

$$
\begin{aligned}
\text{(Prediction Error)}_{\text{training}} &= \frac{1}{n}\sum_{i=1}^{n}\left(\boldsymbol{y}_i - \hat{\boldsymbol{y}}_i\right)^2 = \frac{1}{n}\sum_{i=1}^{n}\left(\boldsymbol{y}_i - \left(\hat{\boldsymbol{\beta}}_0 + \hat{\boldsymbol{\beta}}\boldsymbol{X}_i\right)\right)^2 \\
\text{(Prediction Error)}_{\text{test}} &= \frac{1}{n}\sum_{i=1}^{\text{ntest}}\left(\boldsymbol{y}_{i(\text{test})} - \hat{\boldsymbol{y}}_{i(\text{test})}\right)^2 \\
&= \frac{1}{n}\sum_{i=1}^{\text{ntest}}\left(\boldsymbol{y}_{i(\text{test})} - \left(\hat{\boldsymbol{\beta}}_0 + \hat{\boldsymbol{\beta}}\boldsymbol{X}_{i(\text{test})}\right)\right)^2
\end{aligned}
$$

Analysis Results



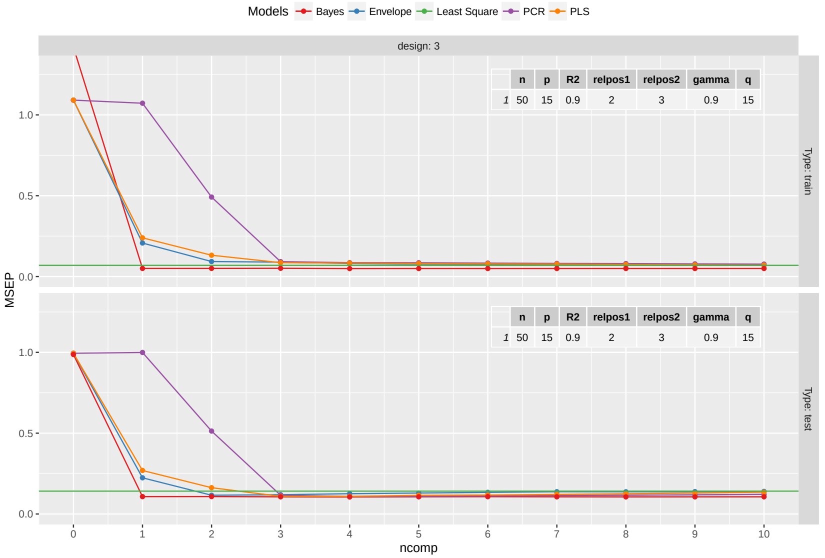
Analysis Results



	n	p	R2	relpos1	relpos2	gamma	q
1	50	40	0.5	1	2	0.5	40

	n	p	R2	relpos1	relpos2	gamma	q
1	50	40	0.5	1	2	0.5	40

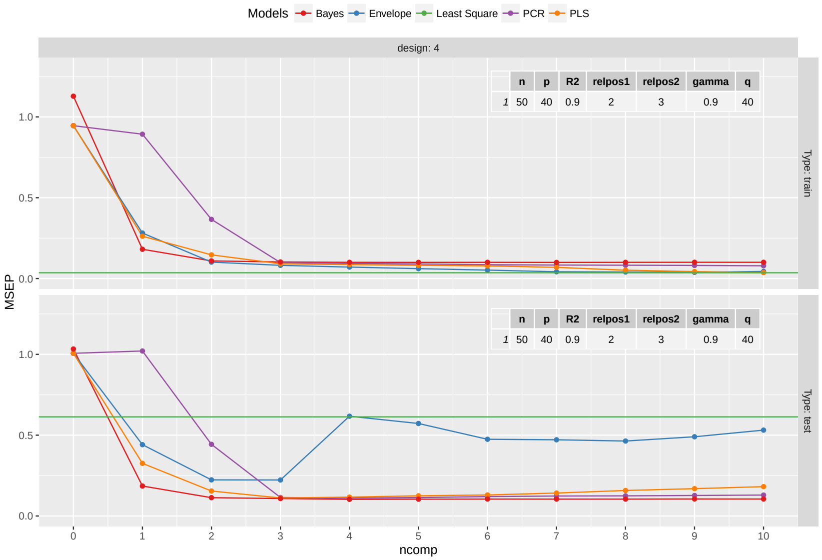
Analysis Results



	n	p	R2	relpos1	relpos2	gamma	q
1	50	15	0.9	2	3	0.9	15

	n	p	R2	relpos1	relpos2	gamma	q
1	50	15	0.9	2	3	0.9	15

Analysis Results



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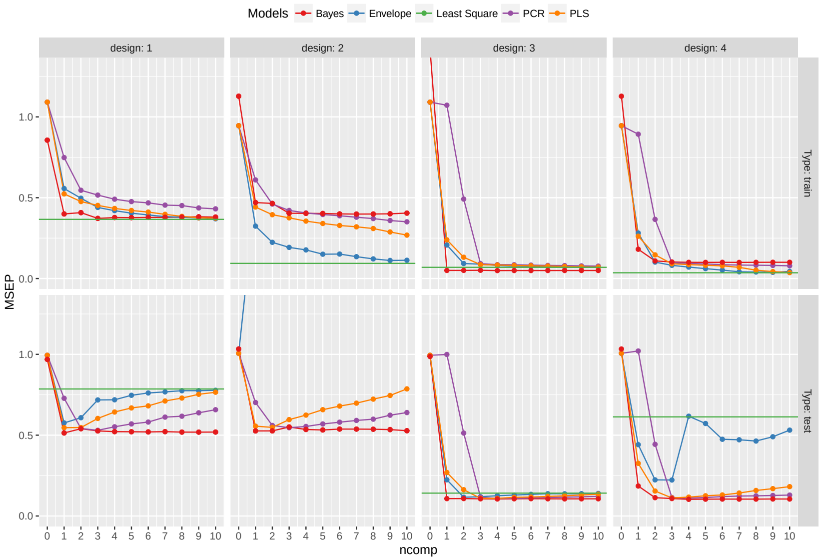

Conclusion

- New methods – Envelope and Bayes, as they claim, are performing better than algorithmic approach of PLS
- However, the performance of MLE approach of Envelope is not satisfactory when number of variable is large
- In the case of Bayes PLS, the prediction error does not raises noticably (test prediction) after capturing enough information with few components
- This suggests that it is able to find the direction of maximum variation after successive rotations of predictor subspace
- The computation regarding BayesPLS is intensive which will not be fisible in case of wide dataset (very common in genomic data)
- All the models are performing better than the least square solution

References

R Dennis Cook and Xin Zhang. Algorithms for envelope estimation. *Journal of Computational and Graphical Statistics*, 25(1):284–300, 2016.

R Dennis Cook, Bing Li, and Francesca Chiaromonte. Envelope models for parsimonious and efficient multivariate linear regression. *Statistica Sinica*, pages 927–960, 2010.

RD Cook, IS Helland, and Z Su. Envelopes and partial least squares regression. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 75(5):851–877, 2013.

Sijmen De Jong. Simpls: an alternative approach to partial least squares regression. *Chemometrics and intelligent laboratory systems*, 18(3): 251–263, 1993.

Inge S Helland. Partial least squares regression and statistical models. *Scandinavian Journal of Statistics*, pages 97–114, 1990.

Inge S Helland. Some theoretical aspects of partial least squares regression. *Chemometrics and Intelligent Laboratory Systems*, 58(2):97–107, 2001.

Inge S Helland, Solve Saebø, Ha Tjelmeland, et al. Near optimal prediction from relevant components. *Scandinavian Journal of Statistics*, 39(4): 695–713, 2012.

Tormod Naes and Inge S Helland. Relevant components in regression. *Scandinavian journal of statistics*, pages 239–250, 1993.

Solve Sæbø, Trygve Almøy, and Inge S Helland. simrel—a versatile tool for linear model data simulation based on the concept of a relevant subspace and relevant predictors. *Chemometrics and Intelligent Laboratory Systems*, 146:128–135, 2015.

Herman Wold. Partial least squares. *Encyclopedia of statistical sciences*, 1985.