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

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Overview

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

- PLS **Population Model** [Helland, 1990] which further discussed by [Naes and Helland, 1993, Helland, 2001]

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- Cook et al. [2013] said that PLS is fundamentally an envelope in the population model

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- 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 $\epsilon \sim \text{NID}(0, \sigma^2)$

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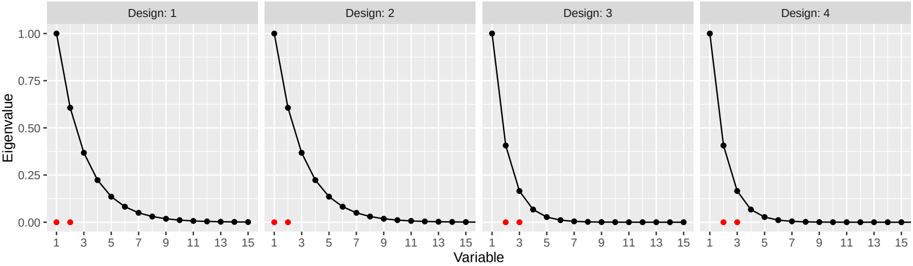
Envelope (MLE)	Bayes
* Estimation using Maximum Likelihood	* Estimation through MCMC approach with rotation of relevant space
* Can not be used when predictor is larger than observations	* Heavy Computation when p is large

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



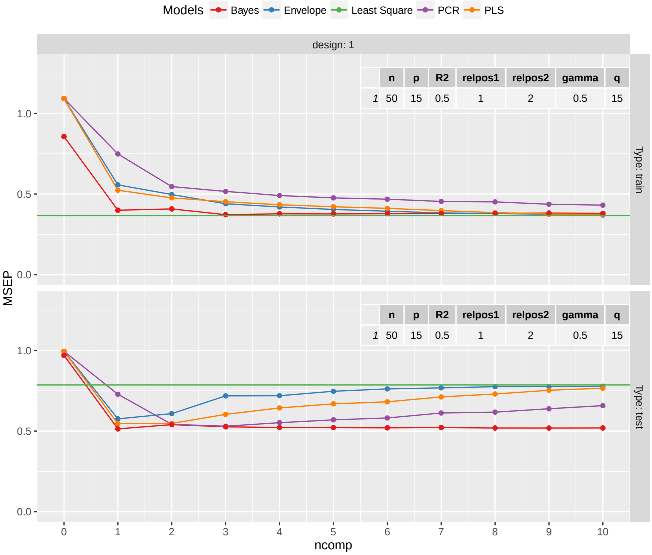
- When Relevant components are at the position of high eigenvalues, the situation is easier to model
- When Relevant components are at the position of low eigenvalues, for example 5, 10, then the most variation present in X are not relevant for Y and this will become a very difficult situation.

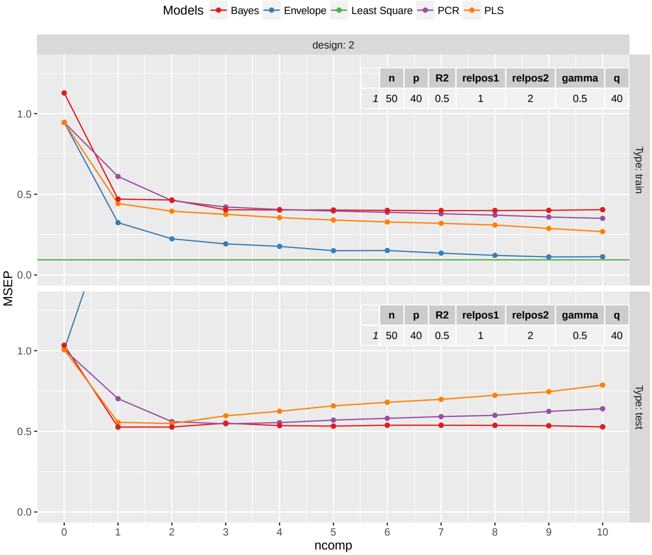
Model assessment

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,

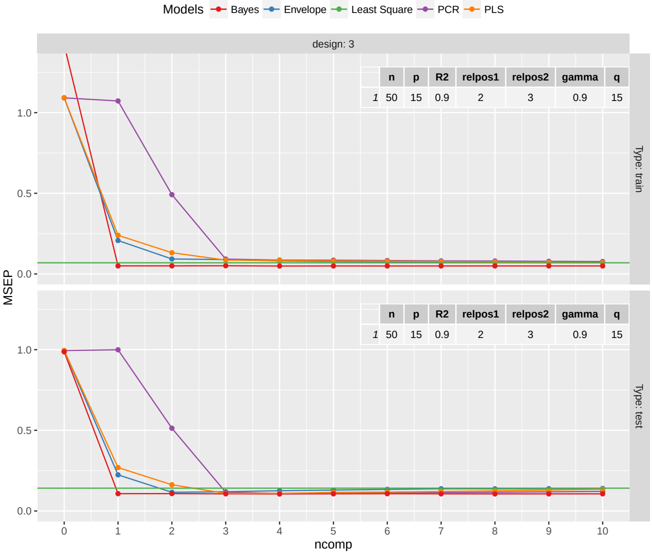
$$
\begin{aligned}
(\text{Prediction Error})_{\text{training}} &= \frac{1}{n}\sum_{i=1}^{n}\left(\boldsymbol{y}_i - \hat{\boldsymbol{y}}_i\right)^2 = \frac{1}{n}\sum_{i=1}^{n}\left(\boldsymbol{y}_i - \left(\hat{\boldsymbol{\beta}}_0 + \hat{\boldsymbol{\beta}}\boldsymbol{X}_i\right)\right)^2 \\
(\text{Prediction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

Analysis Results




Models Bayes Envelope Least Square PCR PLS
design: 2
n p R2 relpos1 relpos2 gamma q
1 50 40 0.5 1 2 0.5 40
Type: train
Type: test
MSEP
1.0
0.5
0.0
0 1 2 3 4 5 6 7 8 9 10
ncomp

Analysis Results



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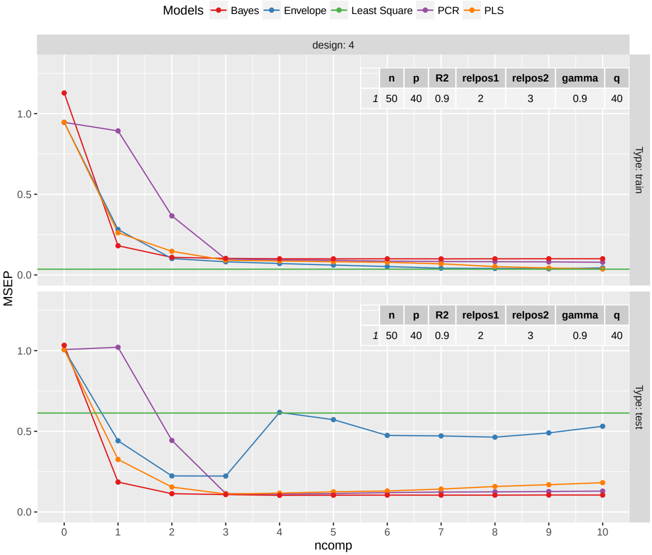

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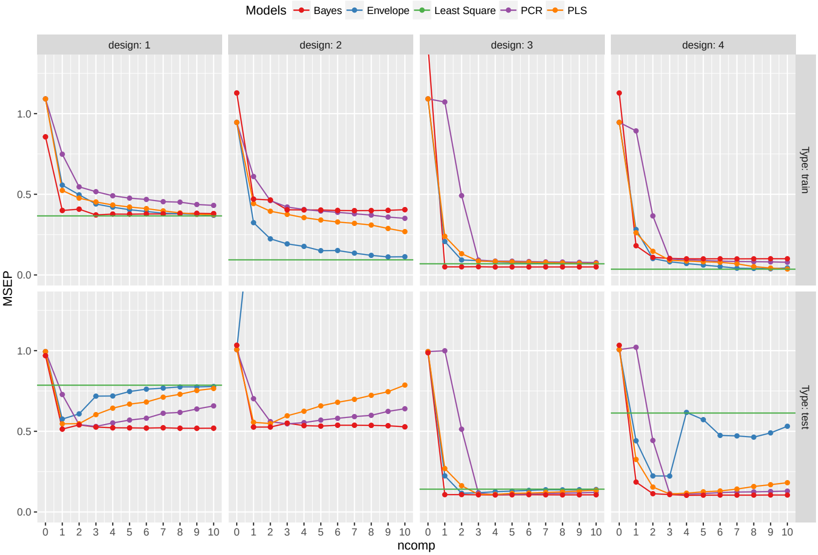

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- All the models are performing better than the least square solution


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