PhD Midway Seminar

Simulation Tool and its application

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Introduction

My PhD Plan

PhD Program	
Phase 1	Make a simulation Tool
Phase 2	Apply it for comparing different estimation Methods
Phase 3	Extend the simulation tool for model with background information
Phase 4	Apply it to test multi-matrix extension of PLS models such as LPLS and UPLS

- Make Simulation Tools for multi-response linear model data
- Using the tool, compare various **estimation techniques** and **understand** them
- **Extend** the simulation tool incorporating model with **background information**
- Apply this extended tool to test multi-matrix extension of partial least square (PLS) models such as LPLS and UPLS (both uses background information about X and Y for analysis)

What I learn

- Advanced Multivariate Model and technique to analyze it
- Programming concept for developing statistical packages and applications for various statistical methods
- Extending and improving existing methods in statistics
- And, obviously, to properly document what I have done

Today’s Special

Today I will talk about:

- Simulation tool (simulatr) we are building
- A comparative study of various estimation techniques by simulating linear model data using simulatr

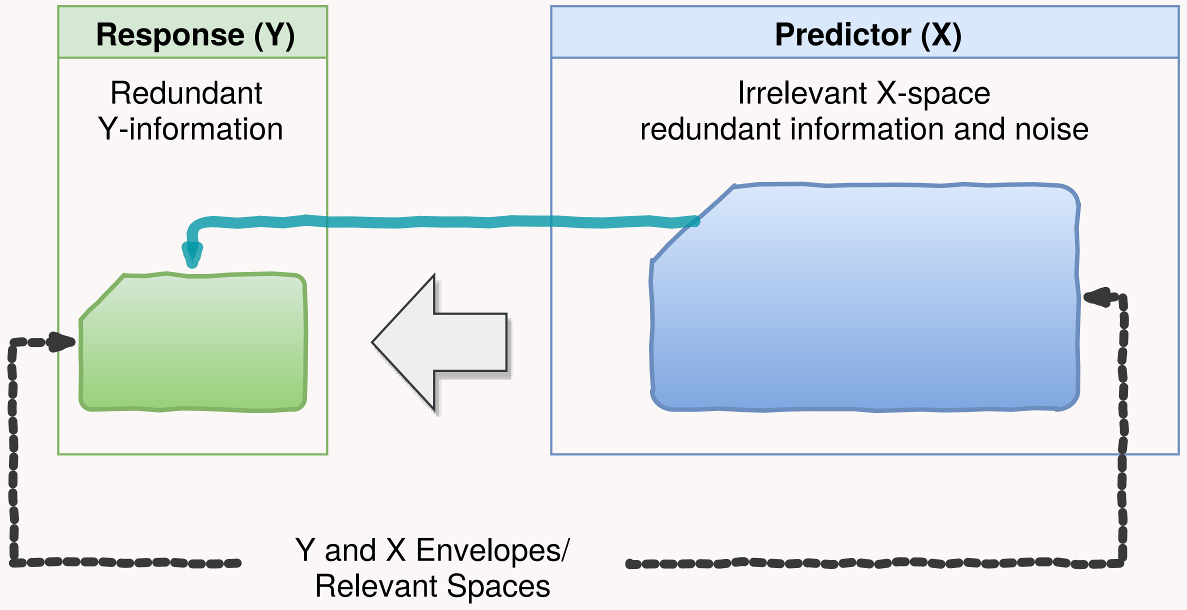
simrel-m: A versatile tool for simulating multi-response linear model data

Overview

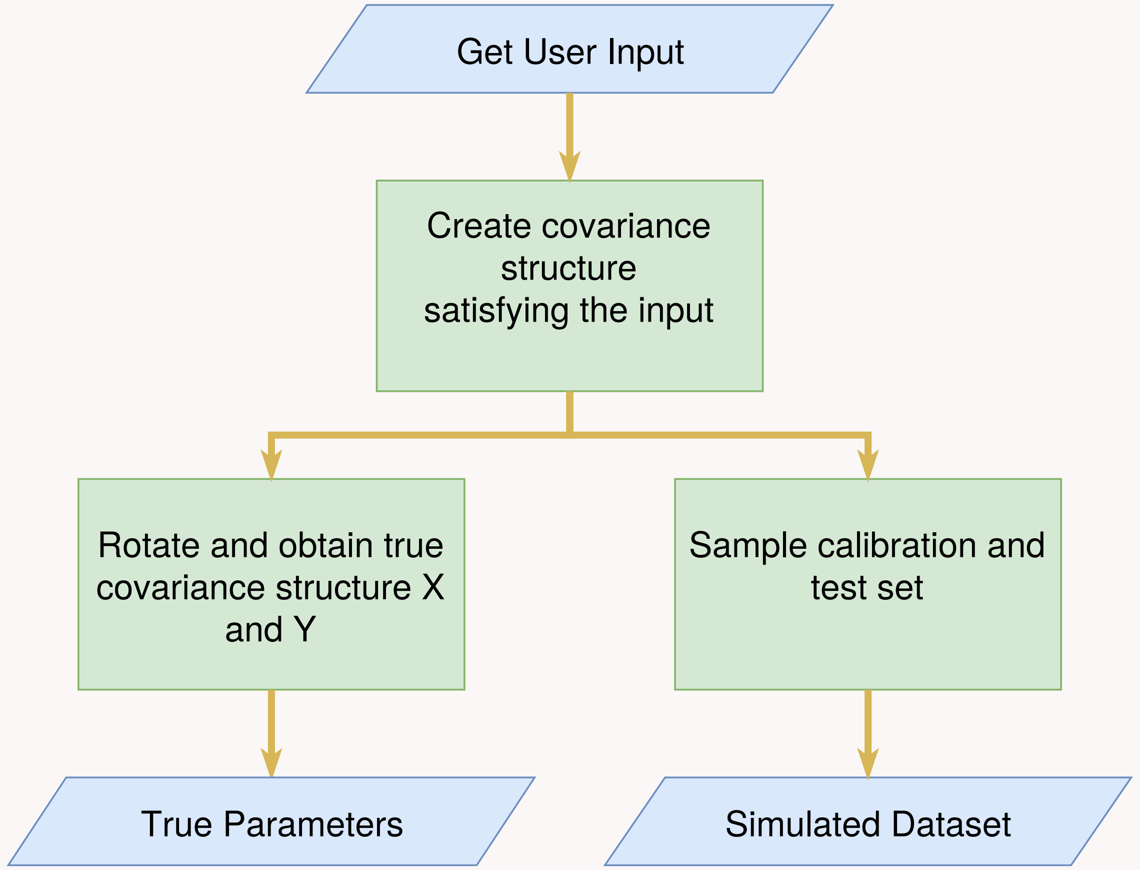
simrel-M is an extension of simrel (Sæbø, Almøy, & Helland, 2015) r-package for simulating multi-response data

- Uses the idea of reduction of random regression model by separating latent space of $\mathbf{X}$ into subspaces that is relevant and irrelevant for predicting each response
- The underlying concept is based on reparameterizing the population model,

$$\mathbf{Y} = \boldsymbol{\mu}_Y + \mathbf{B}^t\left(\mathbf{X} - \boldsymbol{\mu}_X\right) + \boldsymbol{\epsilon}, \text{ where } \boldsymbol{\epsilon} \sim N(0, \boldsymbol{\Sigma}_{Y|X})$$



Underlying procedure



- Collect population input parameter from users such as: number of variables, coefficient of determination and the position of relevant components
- Make a covariance matrix satisfying input parameters
- Rotate the covariance matrix orthogonally
- Sample calibration and validation sets

A comparative study of different estimation methods using simulated data

Overview

Four estimtion methods were considered

Ordinary Least Squares (OLS)

- Although unbiased, suffer highly from multicollinearity
- Widely used and can be used as reference for comparison

Partial Least Squares (PLS)

- Well established and widely used method
- Based on Latent Structure and free of multicollinearity problem

Envelope

- Relatively new method (Cook, Helland, & Su, 2013) and is also based on reduction of regression model
- Based on Maximum Likelihood but works better than OLS in p approaches n

Bayes PLS

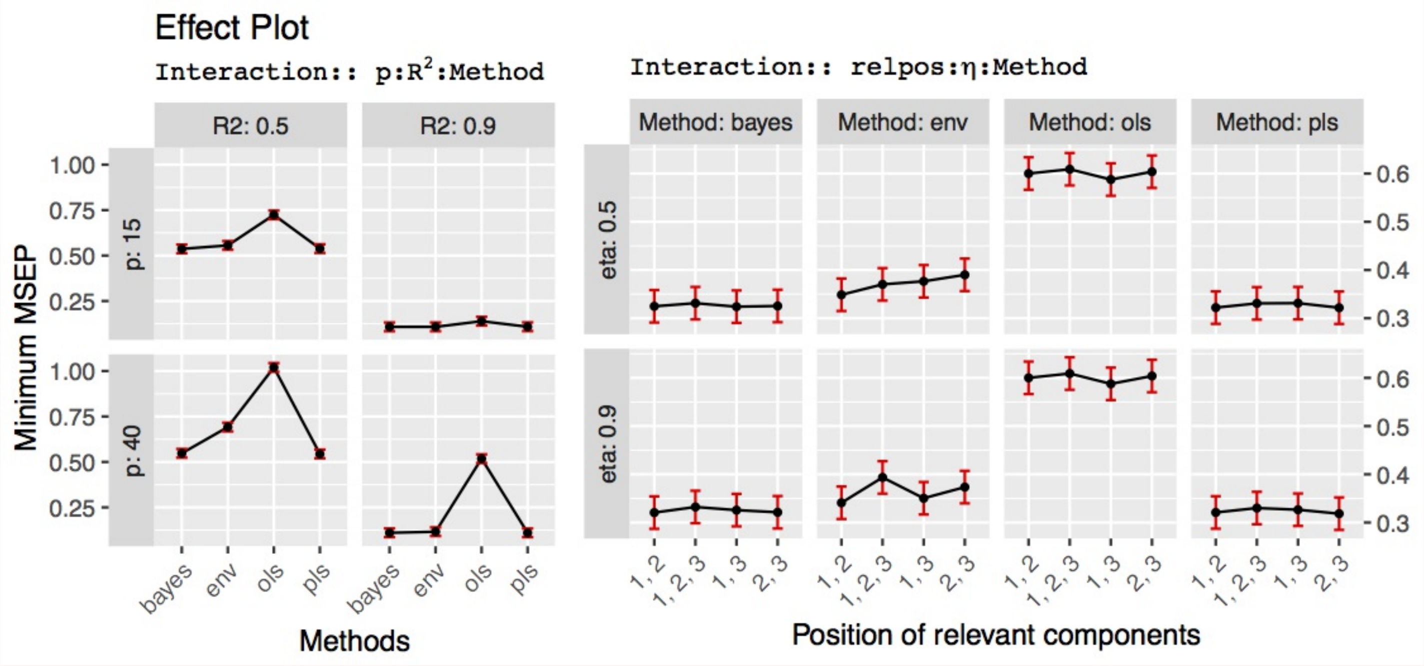
- Bayesian Estimation of regression coefficient
- Promising performance was shown in previous studies (Helland, Sæbø, & Tjelmeland, 2012)

Simulation Design

From the possible combination of following parameter combination, *32* single response calibration sets were simulated with *5* replication of each.

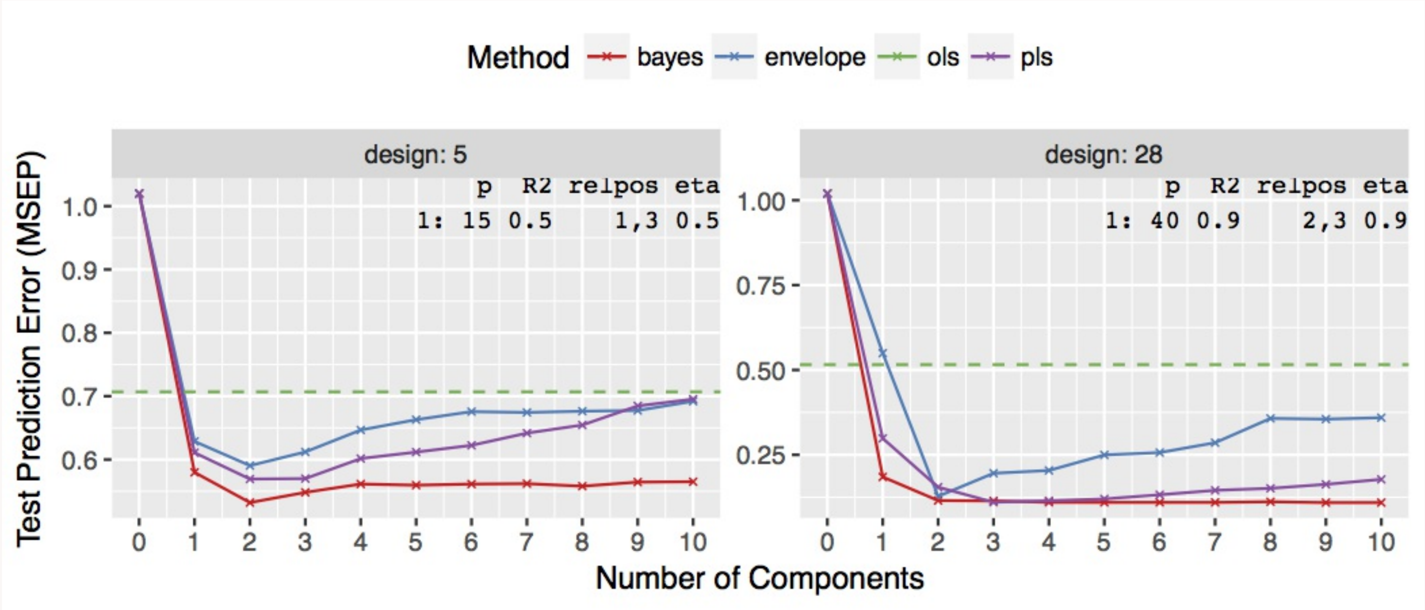
- **Number of sample observations**: *50*
- **Number of predictor variables**: *15* and *40*
- **Coefficient of determination** (R^2): *0.5* and *0.9*
- **Level of multicollinearity**: *0.5* and *0.9*
- **Position of relevant components**: *1* and *2*; *1* and *3*; *2* and *3*; *1*, *2* and *3*

A Systematic Comparison



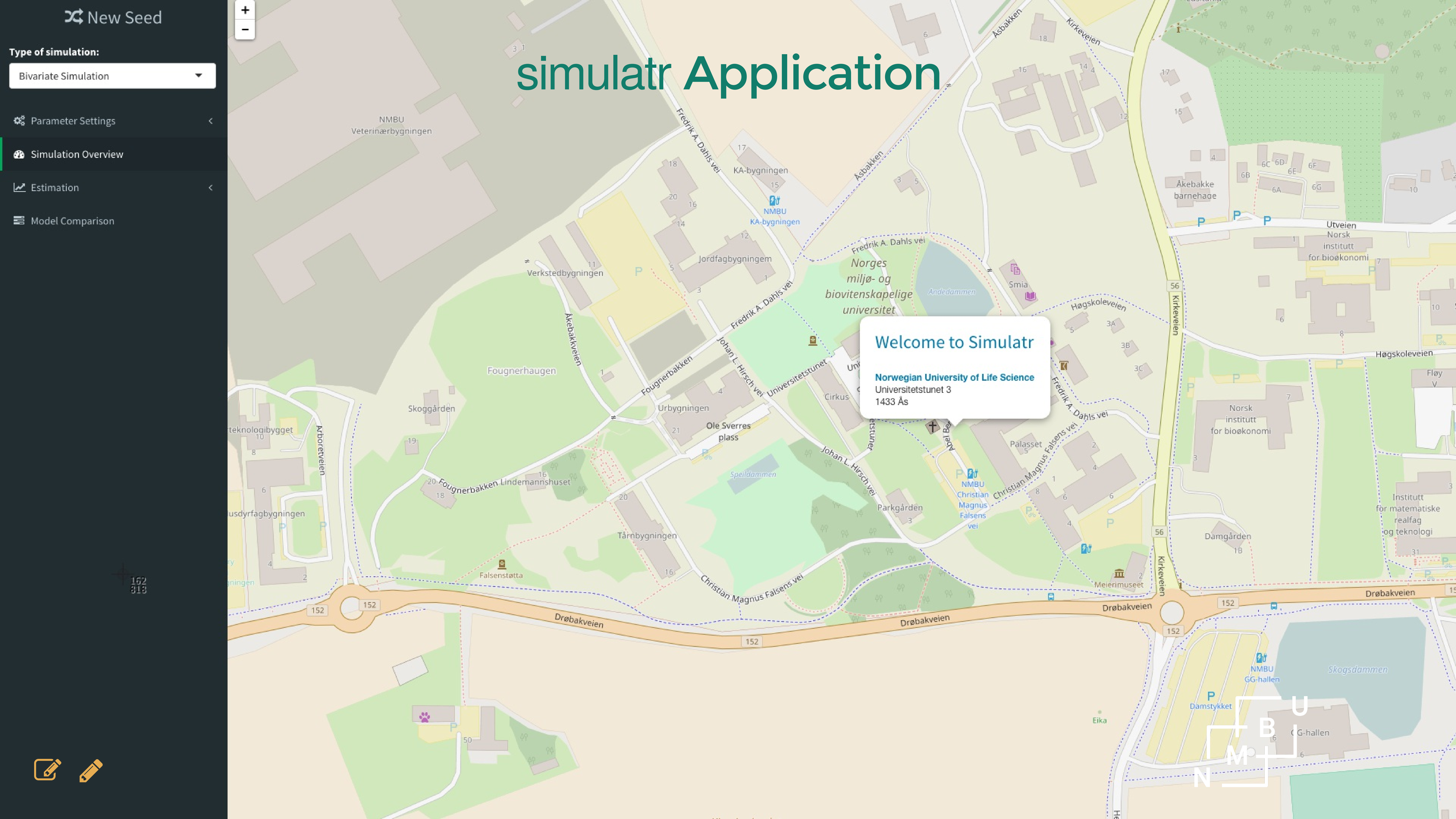
- Bayes PLS has out-performed others methods in all kinds of data
- Envelope has performed better than OLS in all situations and PLS in some situations
- OLS prediction is very poor in noisy data with many predictor variables
- Position of relvant component and the decaying factor of eigenvalue has less impact on prediction in all the models

A Systematic Comparison



- Bayes PLS has approached to its minimum error with very few component and remained low for additional component
- PLS has moderate performance but better than envelope in many situations.
- OLS prediction is poor especially with large number of predictor
- Envelope method captured its minimum error and the error increased with additional components

Demonstration


New Seed
Type of simulation:
Bivariate Simulation
Parameter Settings
Simulation Overview
Estimation
Model Comparison
simulatr Application
Welcome to Simulatr
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多謝
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grazie
спасибо
gracias

References

References

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

Helland, I. S., Sæbø, S., & Tjelmeland. (2012). Near optimal prediction from relevant components. *Scandinavian Journal of Statistics*, *39*(4), 695–713.

Sæbø, S., Almøy, T., & Helland, I. S. (2015). 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.