PhD Midway Seminar

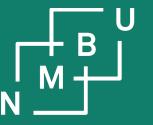
Simulation Tool and its application

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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

Why I am doing this

Important for:

- Research
- Education and
- Method Evaluation





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:

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





A comparative study of different estimation methods using simulated data



Overview

Four estimation methods were considered

Ordinary Least Squares (OLS) Partial Least Squares (PLS)

- Although unbiased, suffer
 Well established and highly from multicollinearity
- Widely used and can be used as reference for comparison
- widely used method
- Based on Latent Structure and free of multicollinearity problem



Overview

Four estimation methods were considered

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 (I. S. Helland, Sæbø,
 & Tjelmeland, 2012)



Simulation Design

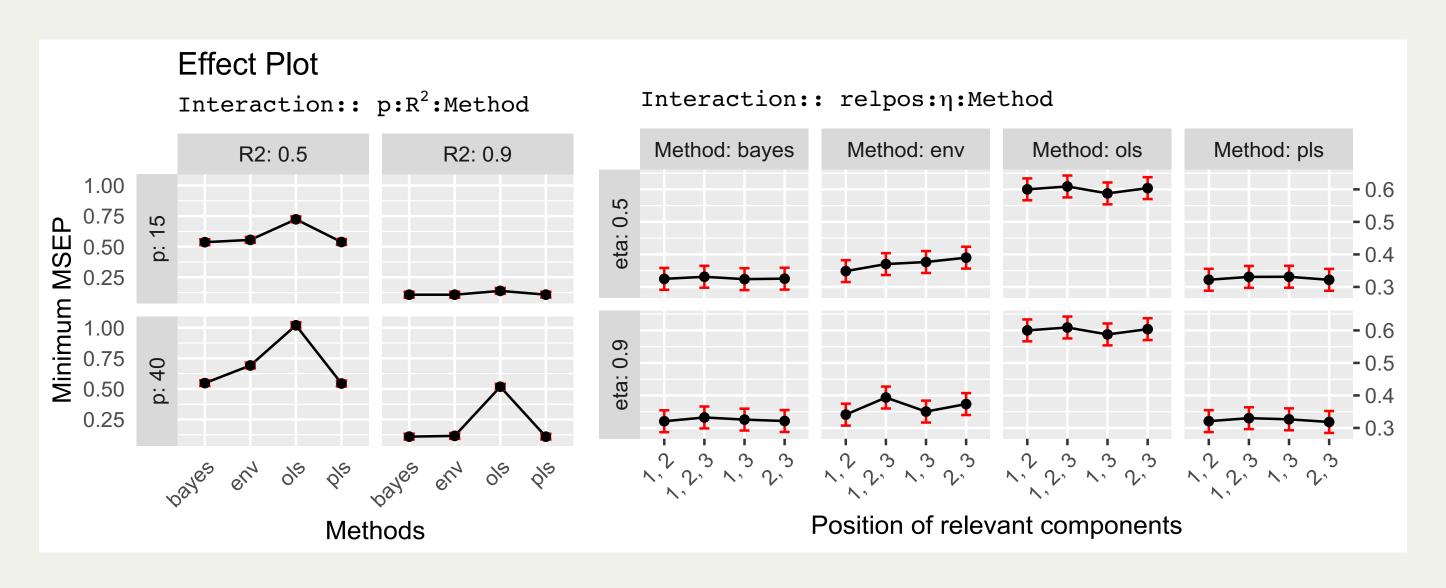
Population Parameters were set as follows:

- 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

From the combination of above parameters, **32** datasets were simulated with **5** replication of each, i.e. **160 datasets** with 5 of them having similar population properties.



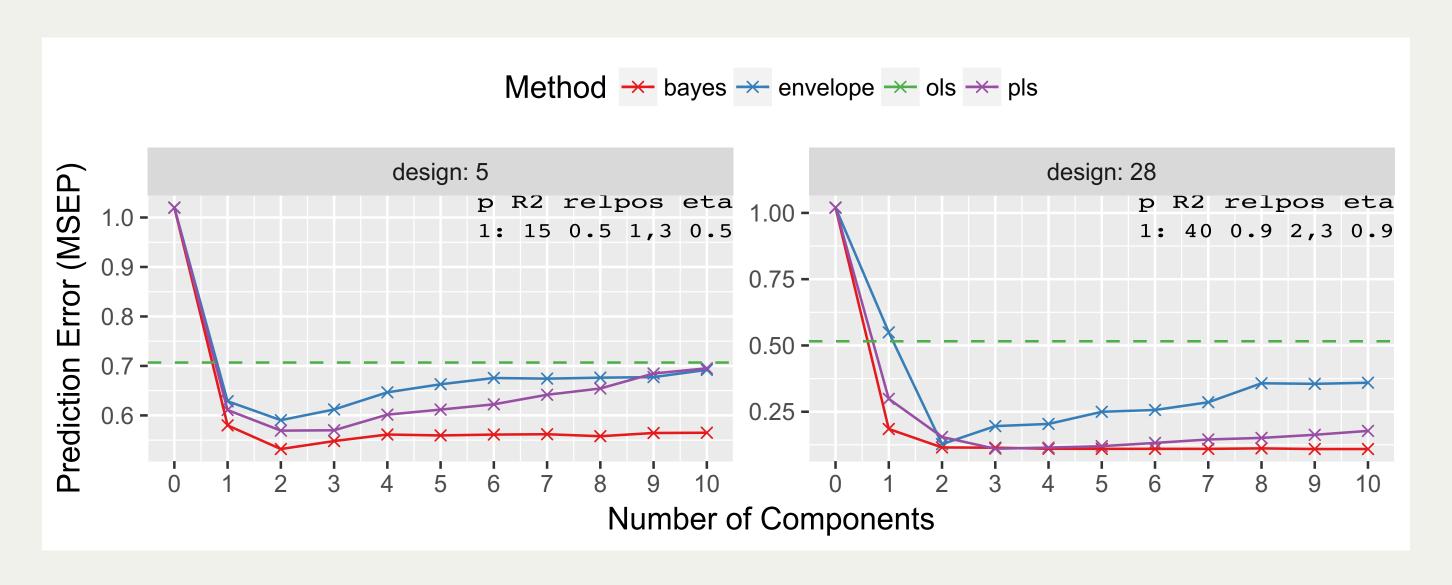
A Systematic Comparison







A Systematic Comparison





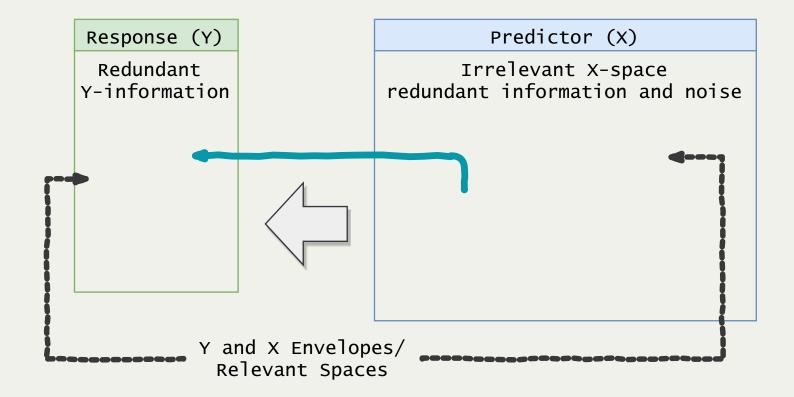


simrel-m: A versatile tool for simulating multi-response linear model data



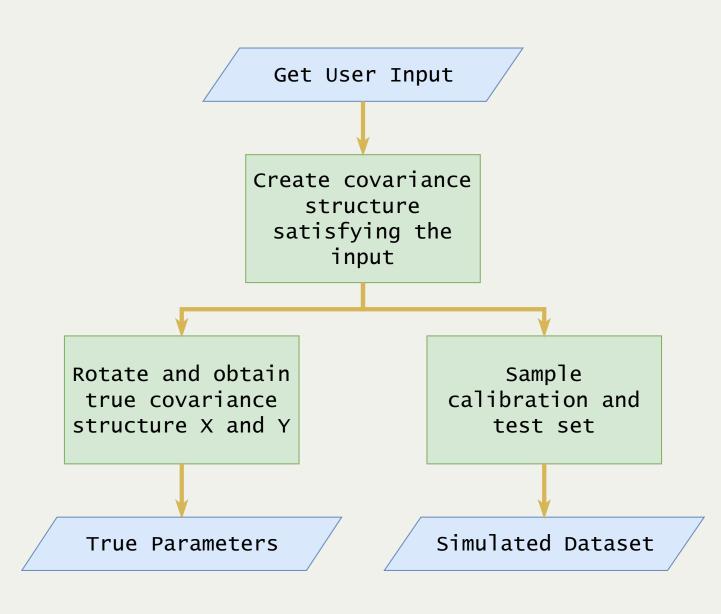
simrel-m

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





How it works



- Collect input parameters from user
- Make a covariance matrix satisfying those input parameters
- Computes true population properties such as regression coefficients
- Sample calibration and validation sets

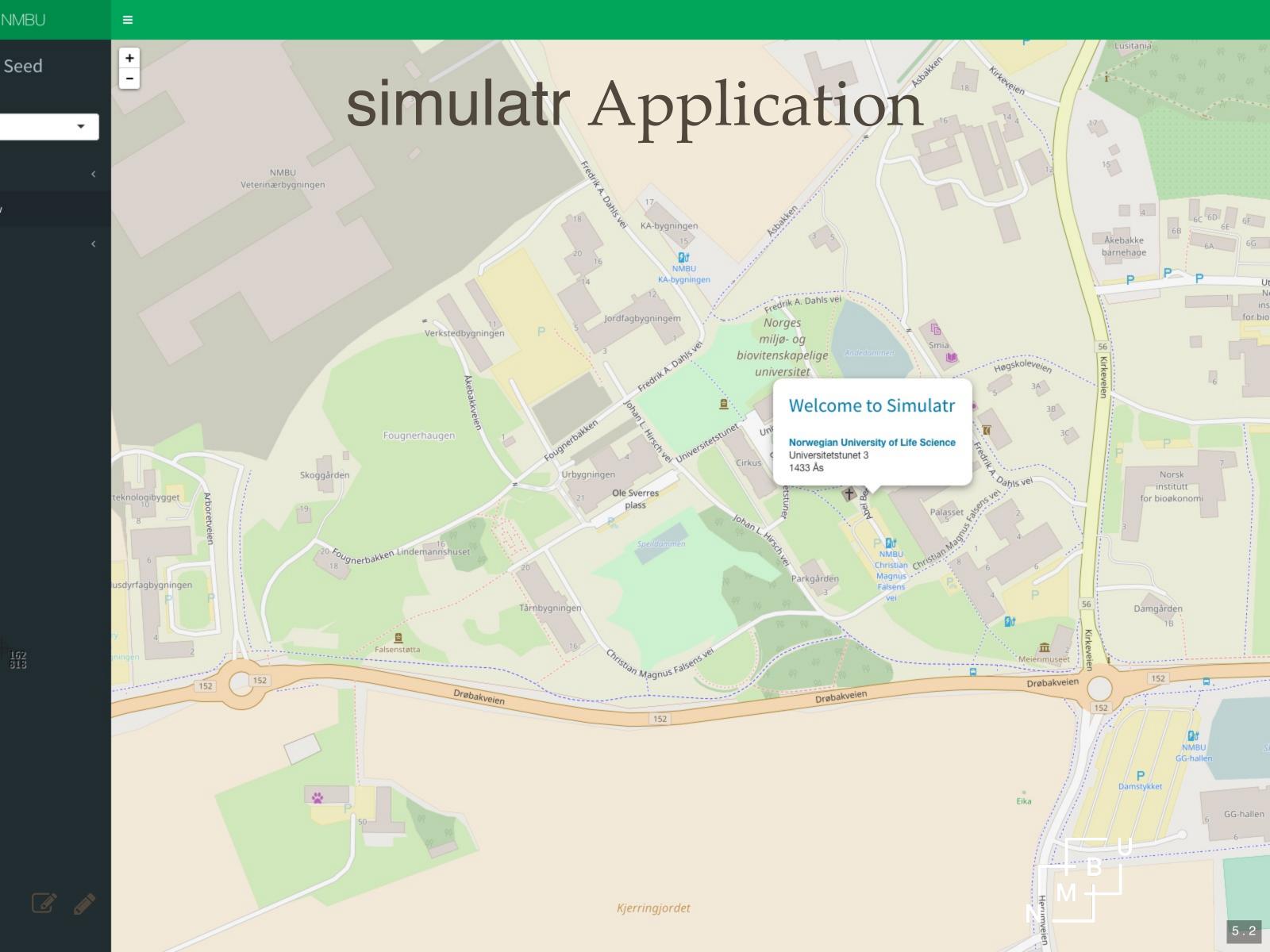




Demonstration

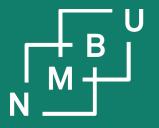






Dakujem GRACIAS teşekkür ederim salamat SUWUN Salamat ASANTE mersi 감사합니다 GRAZAS Ευχαριστώ kiitos merci GRAZZii TAKK Рахмет kiitos sywyn धन्यवाद HVALA DAKUJEM teşekkür ederim hvala kiitos GRACIAS mahalo salamat ASANTE Благодарам спасибо gracias

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.

