Norges miljø- og
biovitenskapelige
universitet

EXPLORATION OF MULTI-RESPONSE MULTIVARIATE METHODS

RAJU RIMAL

20 SEPTEMBER, 2019

Norges miljø- og biovitenskapelige universitet

SUPERVISORS: SOLVE SÆBØ & TRYGVE ALMØY

https://therimalaya.github.io/Dissertation

THE AIM

- Create a versatile ***simulation tool*** capable of simulating multi-response linear-model data with few parameters
- ***Perform*** an extensive ***comparison*** of some new and some established multi-variate methods
- *Explore* the *strength and weaknesses* of these methods in soft (easy to model) and hard (difficult to model) data based on their performance in prediction and estimation

HOW DO YOU EAT AN ELEPHANT?

PAPERS

Contents lists available at ScienceDirect
Chemometrics and Intelligent Laboratory Systems
journal homepage: www.elsevier.com/locate/chemometrics

A tool for simulating multi-response linear model data

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[b] *Prorector, Norwegian University of Life Sciences, Ås, Norway*

Received: 20 November 2017 | Revised: 29 March 2018 | Accepted: 8 April 2018
DOI: 10.1002/cem.3044
RESEARCH ARTICLE
WILEY Journal of CHEMOMETRICS

Model and estimators for partial least squares regression

Inge Svein Helland[1] | Solve Sæbø[2] | Trygve Almøy[2] | Raju Rimal[2]

Comparison of Multi-response Estimation Methods

Raju Rimal[a,*], Trygve Almøy[a], Solve Sæbø[a]

[a] *Faculty of Chemistry and Bioinformatics, Norwegian University of Life Sciences, Ås, Norway*

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Chemometrics and Intelligent Laboratory Systems
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Comparison of multi-response prediction methods

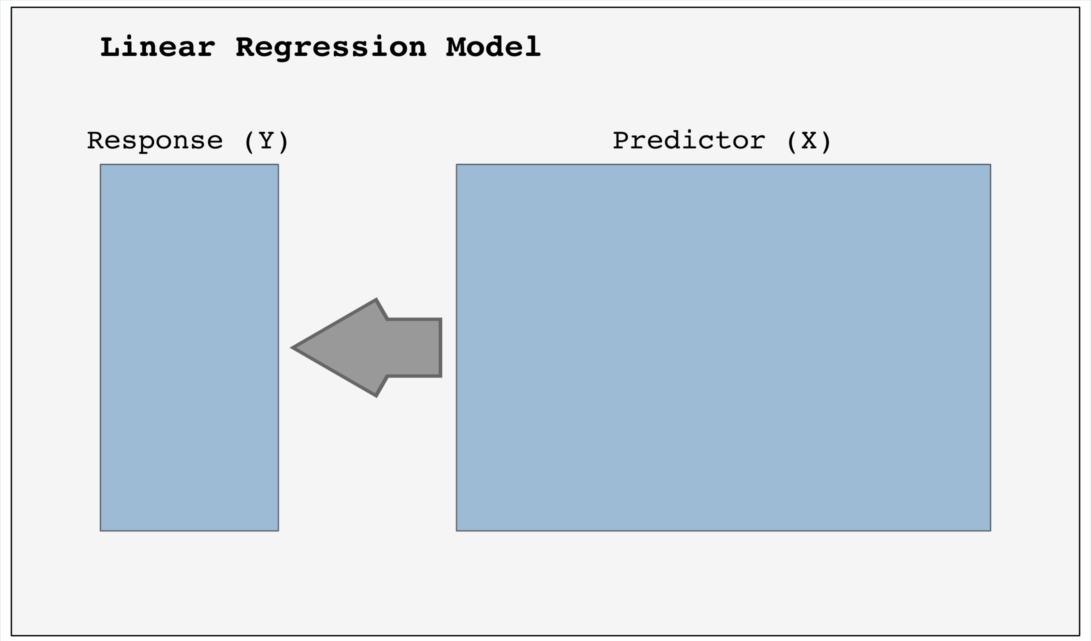
Raju Rimal [a,*], Trygve Almøy [a], Solve Sæbø [b]

[a] *Faculty of Chemistry and Bioinformatics, Norwegian University of Life Sciences, Ås, Norway*
[b] *Norwegian University of Life Sciences, Ås, Norway*

LINEAR REGRESSION MODEL

RELEVANT SPACE AND RELEVANT COMPONENTS

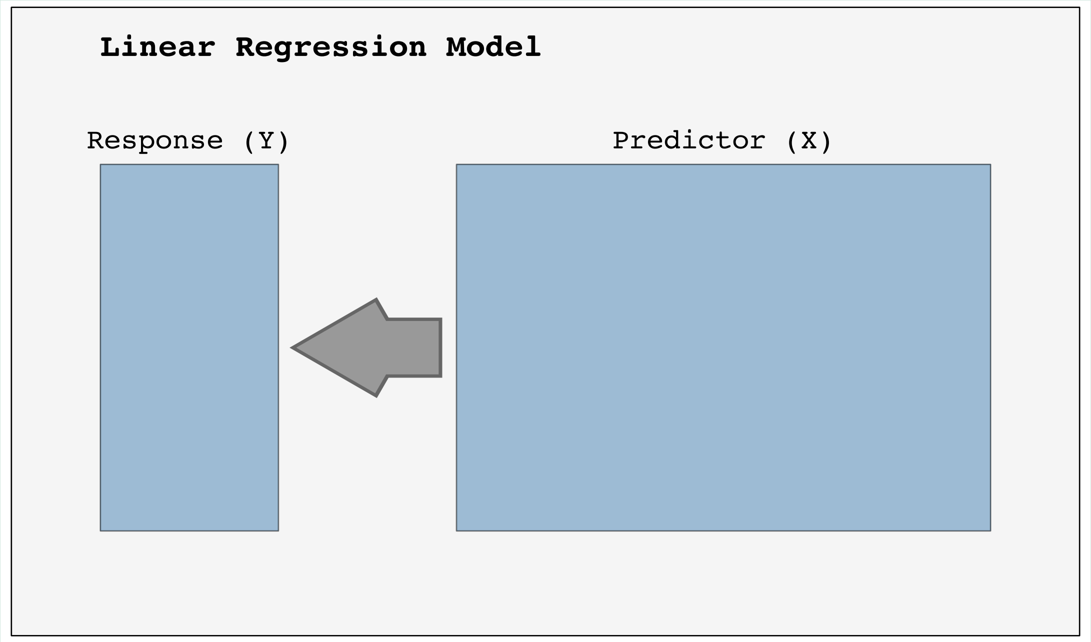
LINEAR REGRESSION MODEL



Linear Regression between $\mathbf{x}$ and $\mathbf{y}$

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

LINEAR REGRESSION MODEL



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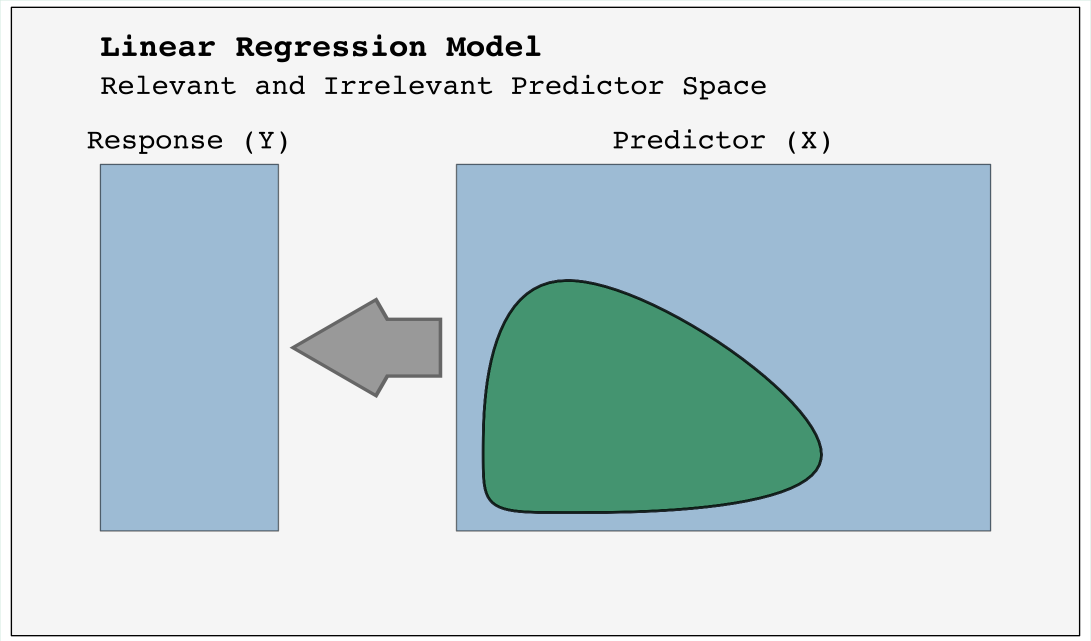
$$\begin{bmatrix} \mathbf{y} \\ \mathbf{x} \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_y \\ \boldsymbol{\mu}_x \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{yy} & \boldsymbol{\Sigma}_{yx} \\ \boldsymbol{\Sigma}_{xy} & \boldsymbol{\Sigma}_{xx} \end{bmatrix} \right)$$

$$\mathbf{y} = \mu_y + \boldsymbol{\beta}^t(\mathbf{x} - \mu_x) + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim \mathrm{N}(0, \Sigma_{x|y})$$

The regression coefficient is the covariance between $\mathbf{x}$ and $\mathbf{y}$ scaled by the variance of $\mathbf{x}$, i.e.

$$\boldsymbol{\beta} = \Sigma_{xx}^{-1}\Sigma_{xy}$$

LINEAR REGRESSION MODEL



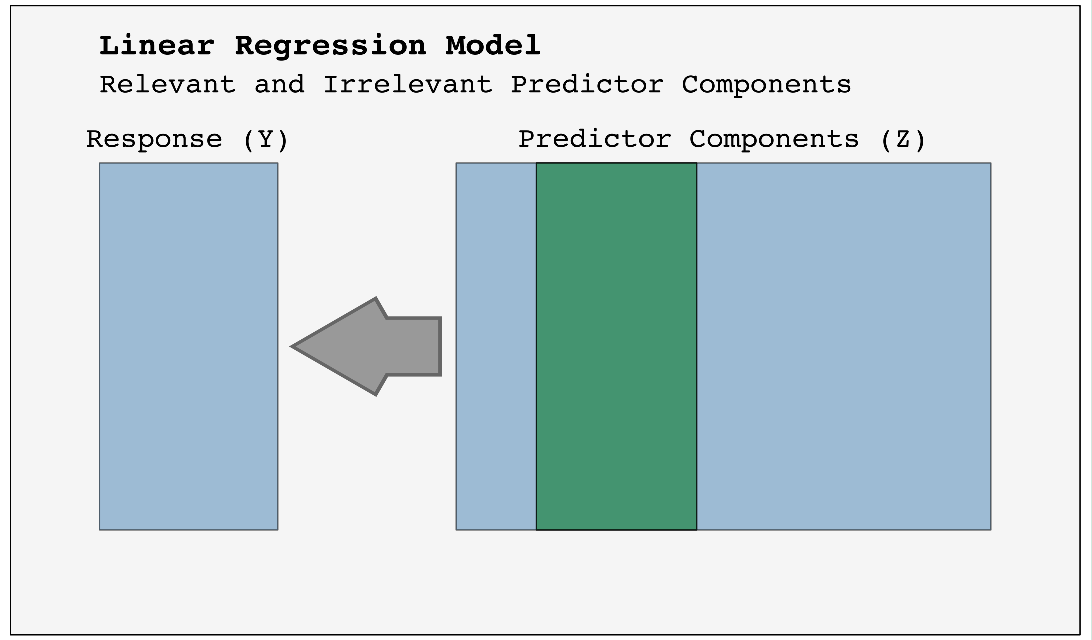
Linear Regression between $\mathbf{x}$ and $\mathbf{y}$

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

$$\mathbf{y} = \mu_y + \boldsymbol{\beta}^t(\mathbf{x} - \mu_x) + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim \mathrm{N}(0, \Sigma_{x|y})$$

- Only a subspace of predictor space is relevant for explaining variation in $\mathbf{y}$

LINEAR REGRESSION MODEL



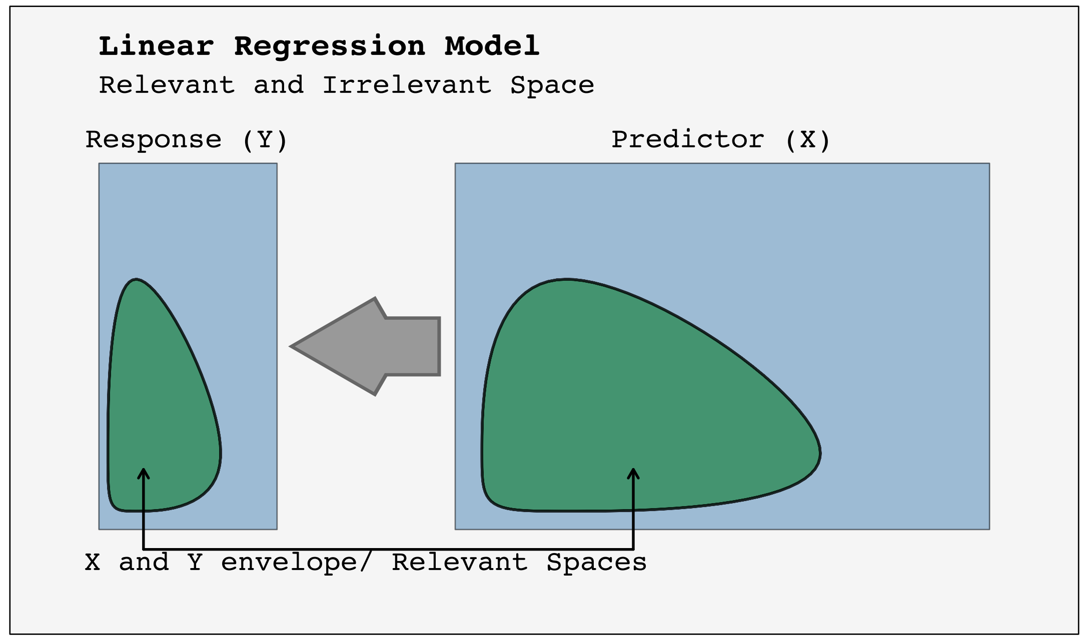
Linear Regression between $\mathbf{x}$ and $\mathbf{y}$

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

$$\mathbf{y} = \mu_y + \boldsymbol{\beta}^t(\mathbf{x} - \mu_x) + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim \mathrm{N}(0, \Sigma_{x|y})$$

- Only a subspace of predictor space is relevant for explaining variation in $\mathbf{y}$
- A subset of latent components that spans this space are the *relevant components*

LINEAR REGRESSION MODEL



Linear Regression between $\mathbf{x}$ and $\mathbf{y}$

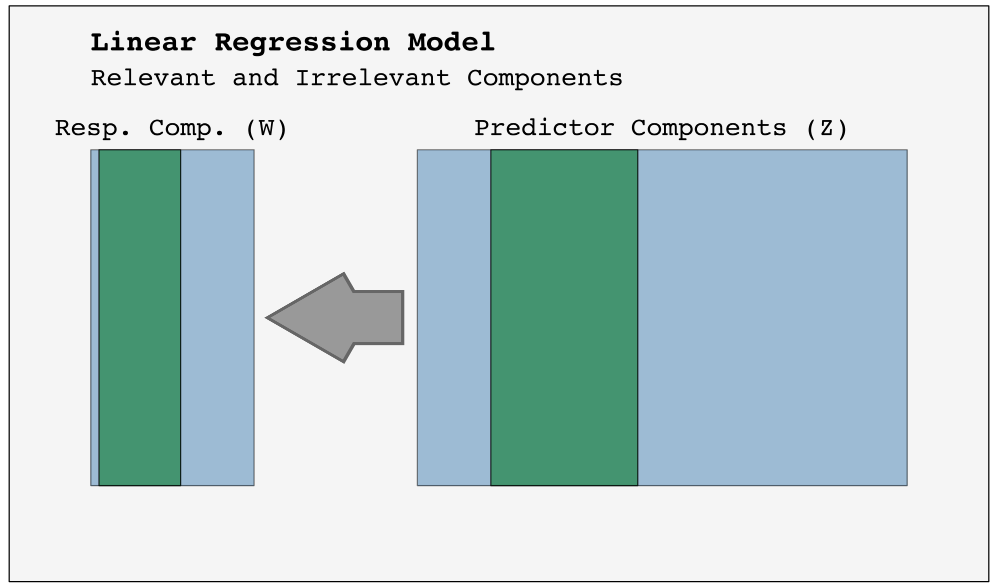
$$\begin{bmatrix}\mathbf{y}\\ \mathbf{x}\end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix}\boldsymbol{\mu}_y\\ \boldsymbol{\mu}_x\end{bmatrix}, \begin{bmatrix}\boldsymbol{\Sigma}_{yy} & \boldsymbol{\Sigma}_{yx}\\ \boldsymbol{\Sigma}_{xy} & \boldsymbol{\Sigma}_{xx}\end{bmatrix}\right)$$

$$\mathbf{y} = \mu_y + \boldsymbol{\beta}^t(\mathbf{x} - \mu_x) + \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim \mathrm{N}(0, \Sigma_{x|y})$$

- Methods like PCR, PLS and Envelopes have used the concept of relevant space
- The concept can also be extended to response space.

SIMREL: A SIMULATION TOOL

- Leveraging the idea, Sæbø, Almøy and Helland (2015) developed a simulation tool called *simrel*



Linear Regression between $\mathbf{z}$ and $\mathbf{w}$ with relevant spaces within them.

$$\mathbf{w} = \mu_w + \boldsymbol{\alpha}^t(\mathbf{z} - \mu_z) + \boldsymbol{\tau}, \quad \boldsymbol{\tau} \sim \mathrm{N}(0, \Sigma^2_{w|z})$$

SIMREL: A SIMULATION TOOL

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BEHIND SIMREL

1. Construct a covariance matrix of $\mathbf{w}$ and $\mathbf{z}$

SIMREL: A SIMULATION TOOL

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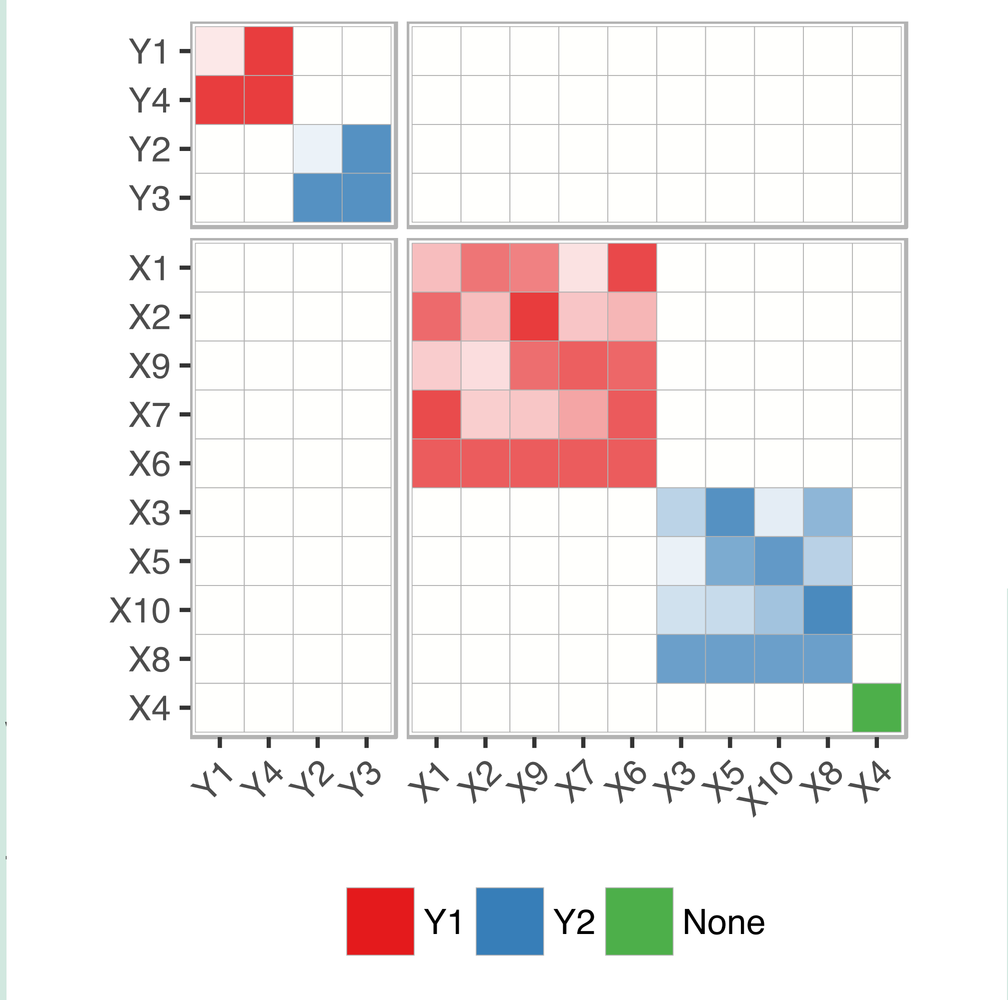
BEHIND SIMREL

1. Construct a covariance matrix of $\mathbf{w}$ and $\mathbf{z}$
2. Construct a rotation matrix that makes our criteria satisfy



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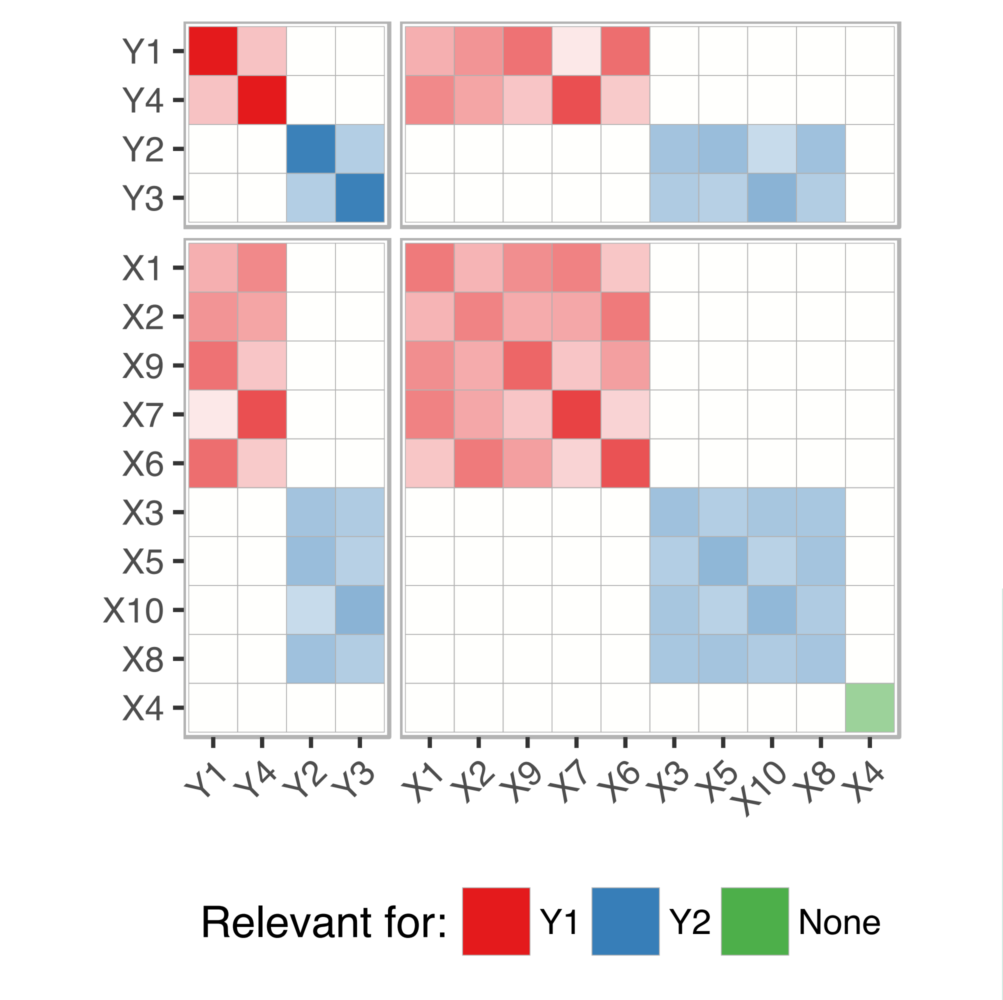
BEHIND SIMREL

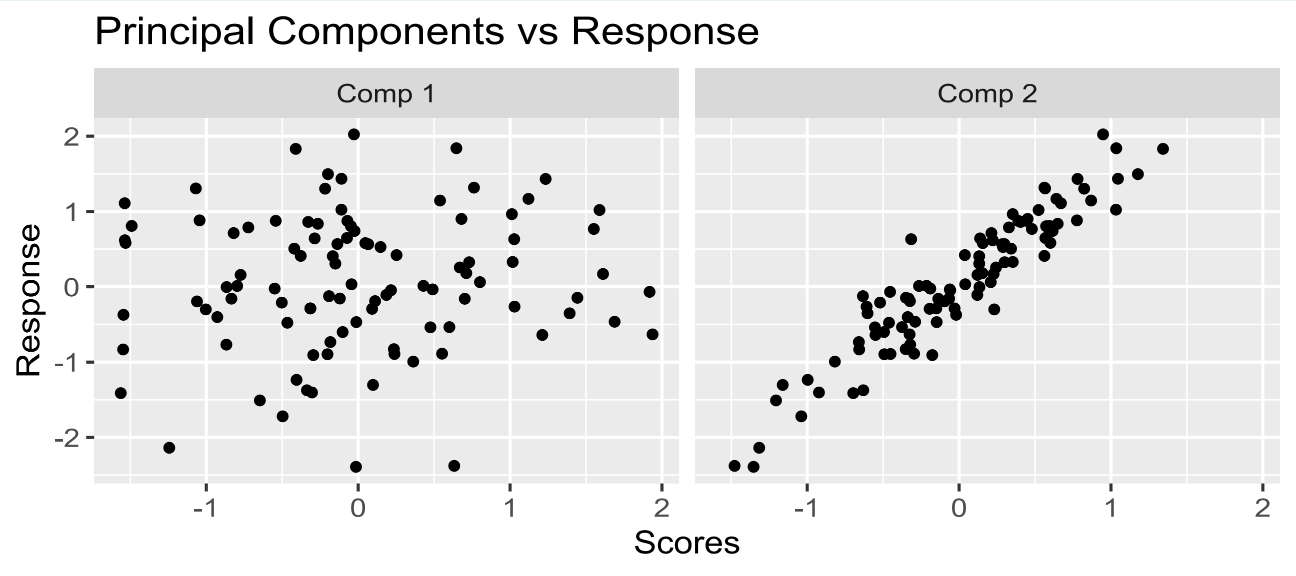
1. Construct a covariance matrix of $\mathbf{w}$ and $\mathbf{z}$
2. Construct a rotation matrix that makes our criteria satisfy
3. Rotate the first by the second and get the true covariance structure for the data to simulate
4. Simulate the data

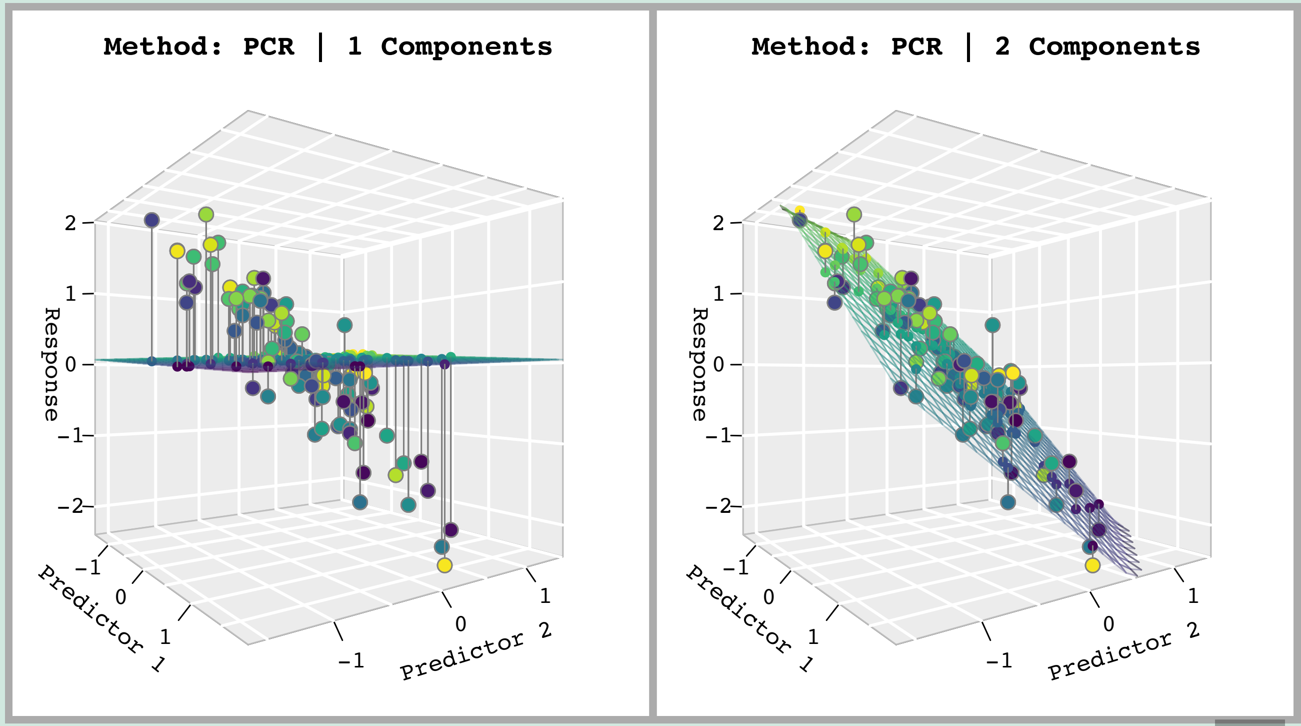


SOME MULTI-VARIATE METHODS AND DESIGN OF EXPERIMENTS

SOME MULTIVARIATE METHODS

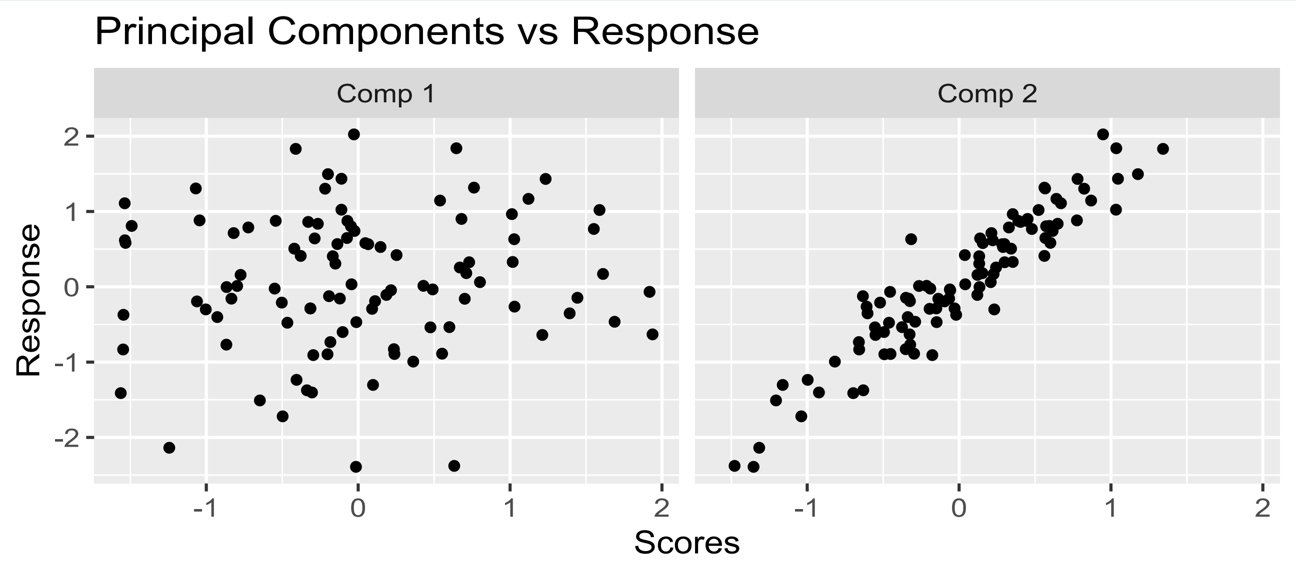
- PRINCIPAL COMPONENT REGRESSION

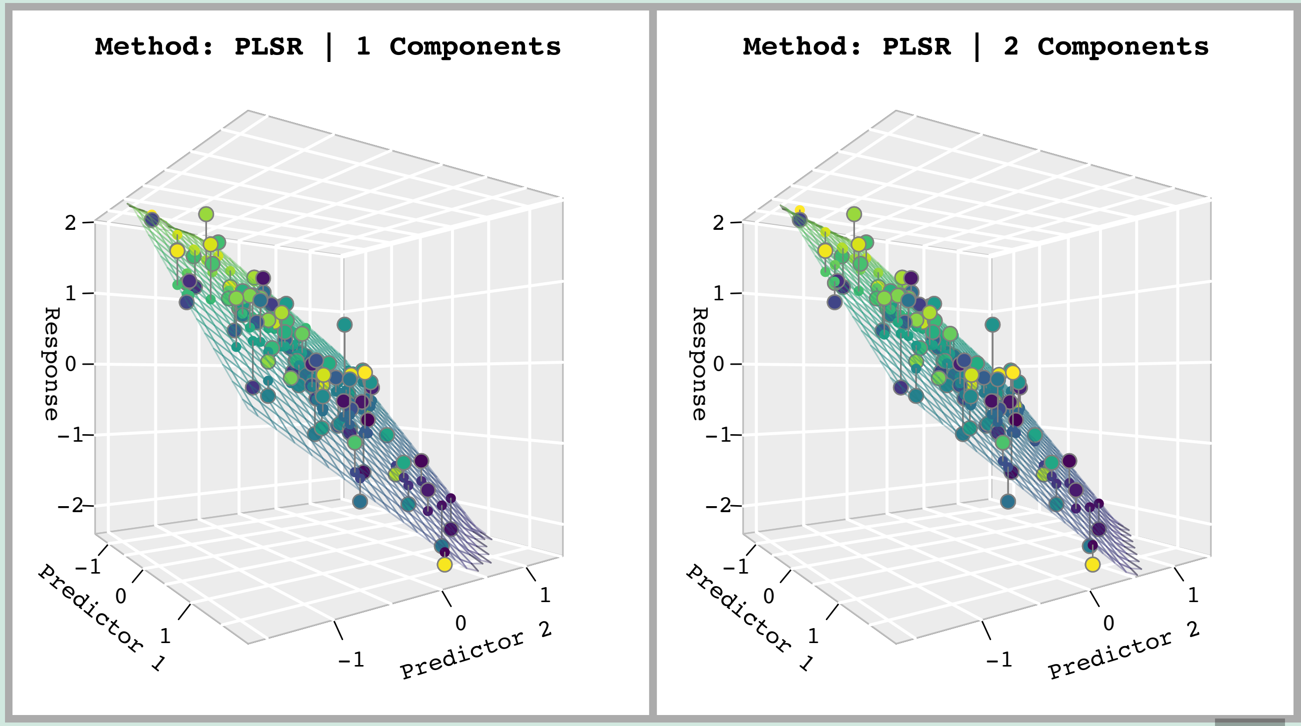




SOME MULTIVARIATE METHODS

- PRINCIPAL COMPONENT REGRESSION
- PARTIAL LEAST SQUARES REGRESSION





SOME MULTIVARIATE METHODS

- ENVELOPES
  - IN RESPONSE

$$Y = \mu_y + \beta(X - \mu_x) + \varepsilon,$$

$$Y = \mu_y + \Gamma\varphi(X - \mu_x) + \varepsilon,$$

$$\Sigma_{Y|X} = \Gamma\Omega\Gamma^T + \Gamma_0\Omega_0\Gamma_0^T$$

SOME MULTIVARIATE METHODS

- ENVELOPES
  - IN RESPONSE
  - IN PREDICTORS

$$Y = \mu_y + \beta(X - \mu_x) + \varepsilon,$$

$$Y = \mu_y + \varphi^T \Phi^T (X - \mu_x) + \varepsilon,$$

$$\Sigma_{XX} = \Phi \Delta \Phi^T + \Phi_0 \Delta_0 \Phi_0^T$$

SOME MULTIVARIATE METHODS

- ENVELOPES
  - IN RESPONSE
  - IN PREDICTORS
  - SIMULTANEOUS

$$
\begin{aligned}
Y &= \mu_y + \beta(X - \mu_x) + \varepsilon, \\
Y &= \mu_y + \Gamma\varphi\Phi^T(X - \mu_x) + \varepsilon, \\
\Sigma_{Y|X} &= \Gamma\Omega\Gamma^T + \Gamma_0\Omega_0\Gamma_0^T \\
\Sigma_{XX} &= \Phi\Delta\Phi^T + \Phi_0\Delta_0\Phi_0^T
\end{aligned}
$$

AN EXAMPLE FROM THE STUDY

EXPERIMENTAL DESIGN

Number of training samples (n)	`n`	50
Number of predictor variables (p)	`p`	15 and 40
Population coefficient of determination (ρ^2)	`R2`	0.5 and 0.9
Position of relevant components	`relpos`	▻ 1, 2 ▻ 2, 3 ▻ 1, 3 and ▻ 1, 2, 3
Decay factor of eigenvalues of Σ_{xx} (γ)	`gamma`	0.5 and 0.9

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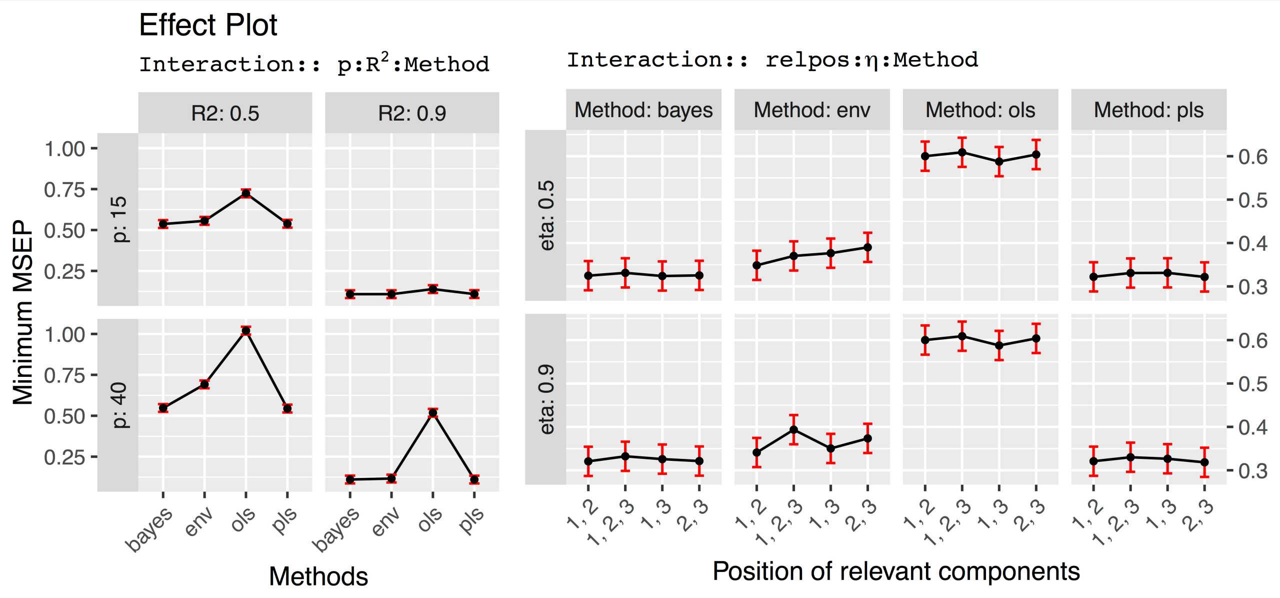

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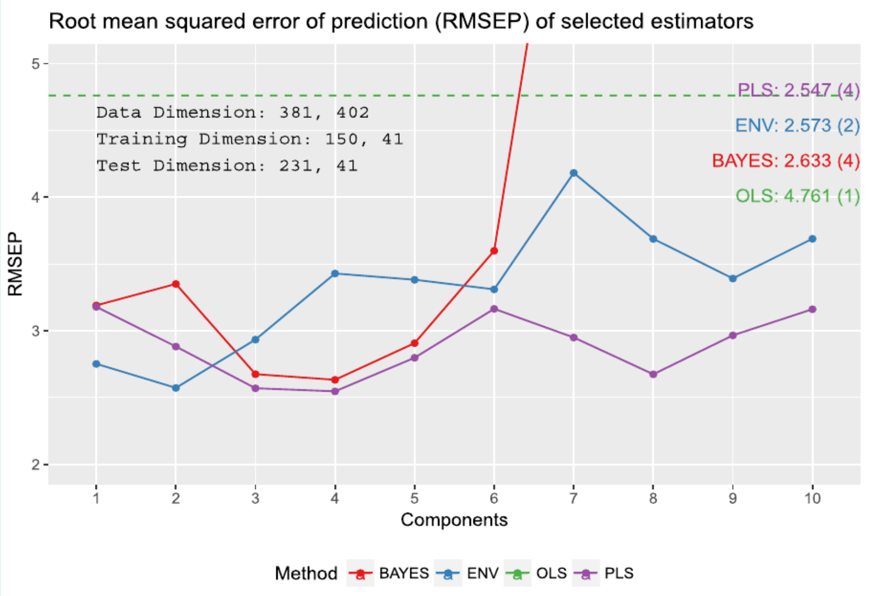
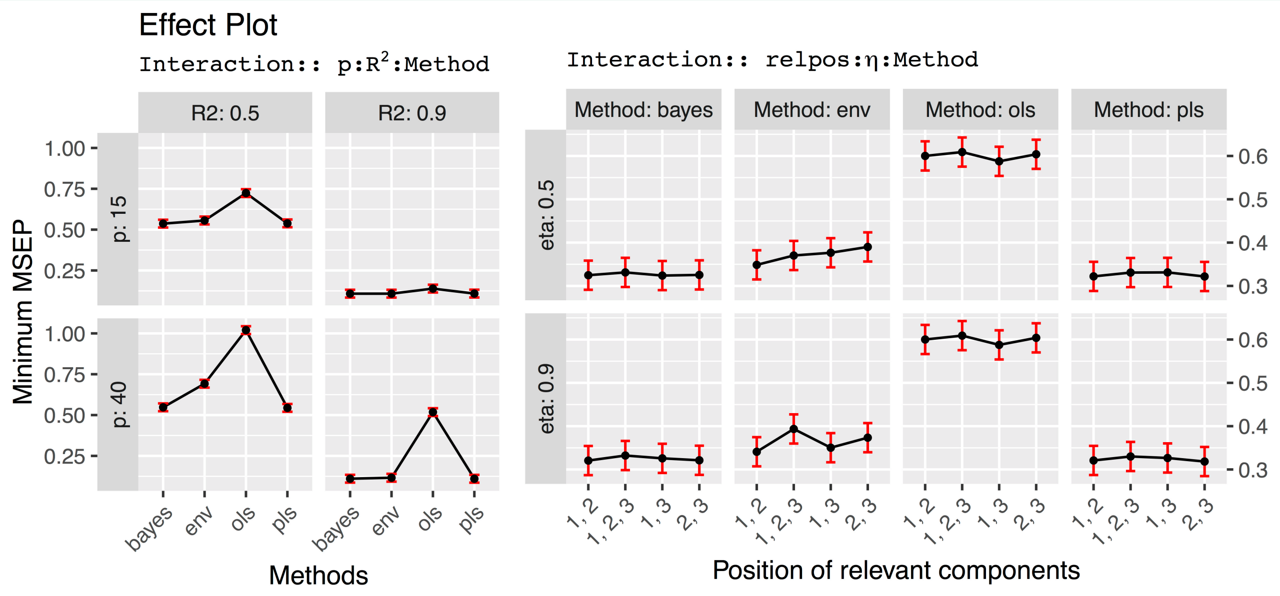
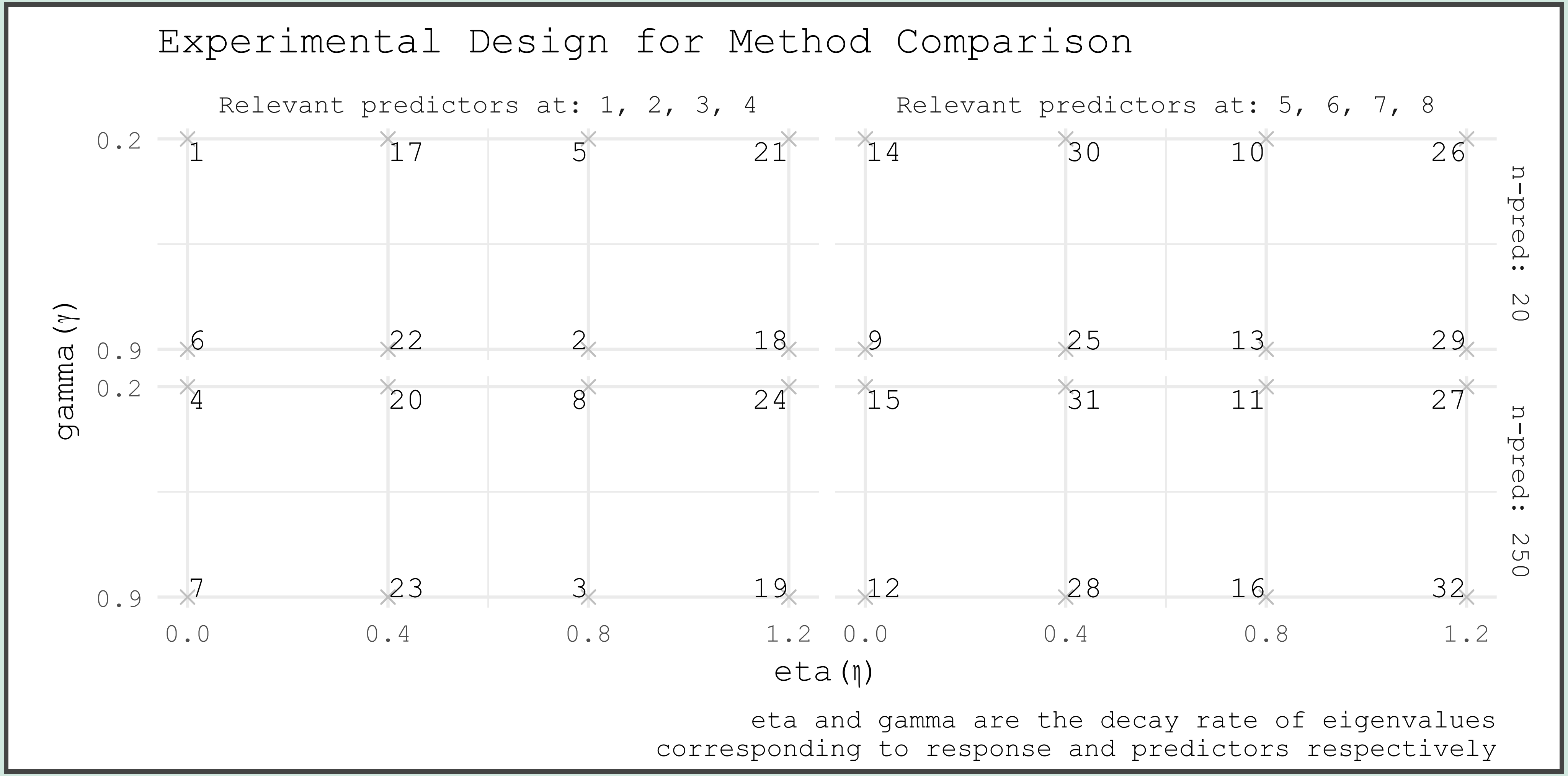




DESIGN OF THE COMPARISON EXPERIMENT

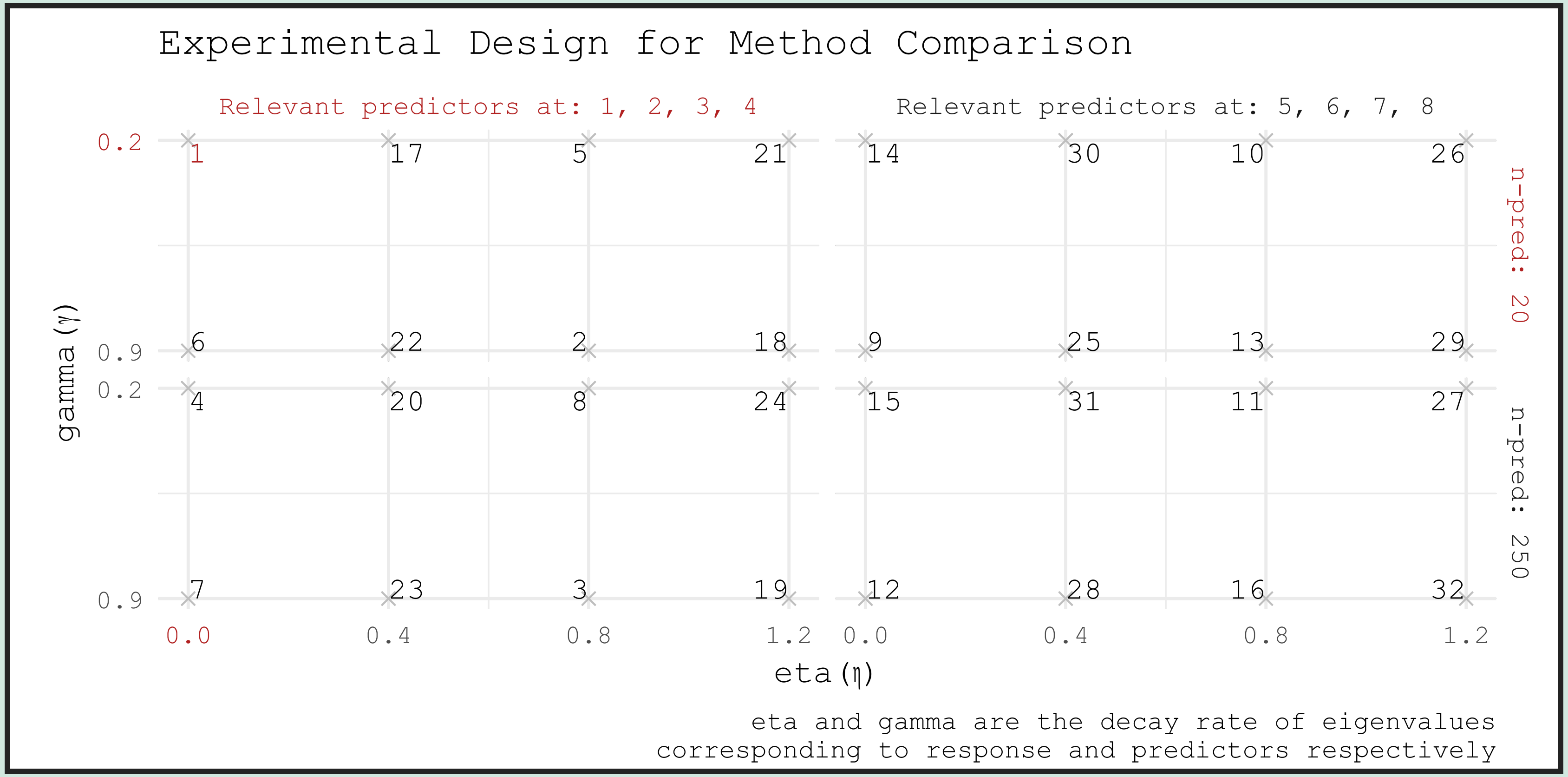


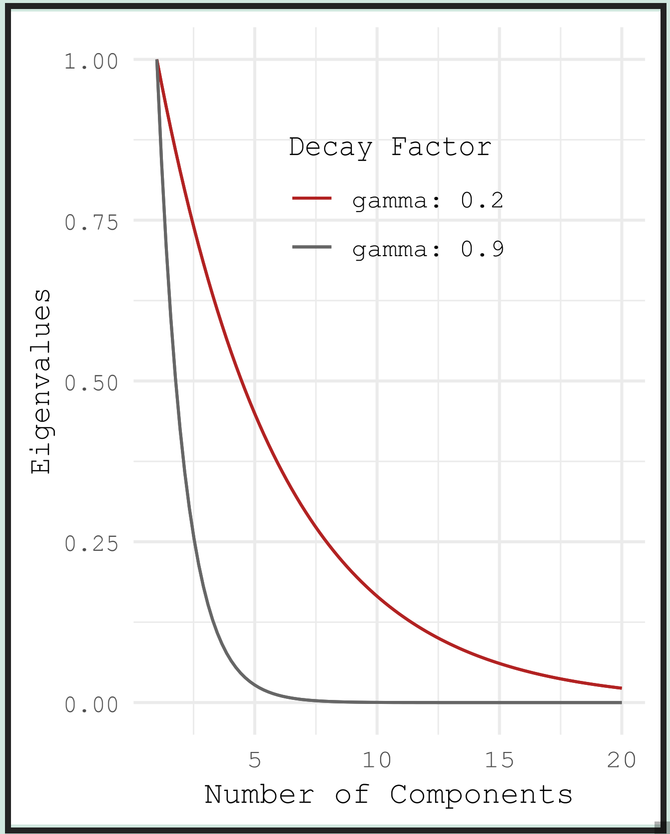
DESIGN OF THE COMPARISON EXPERIMENT

- Small correlation between predictors
- No correlation between responses
- Relevant predictor components at position 1, 2, 3, 4

DESIGN 1

- Number of predictor variables: 20 $n > p$



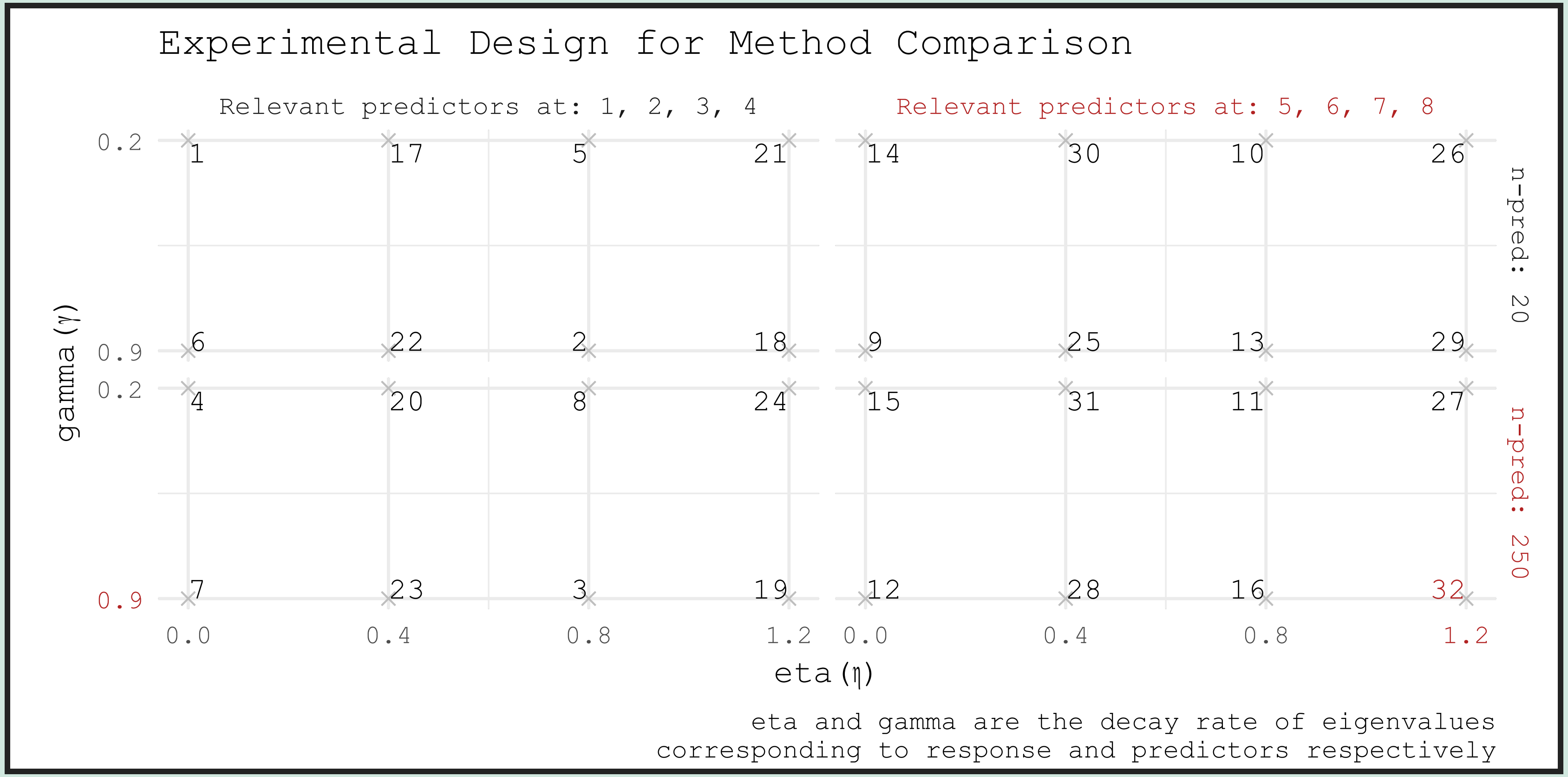


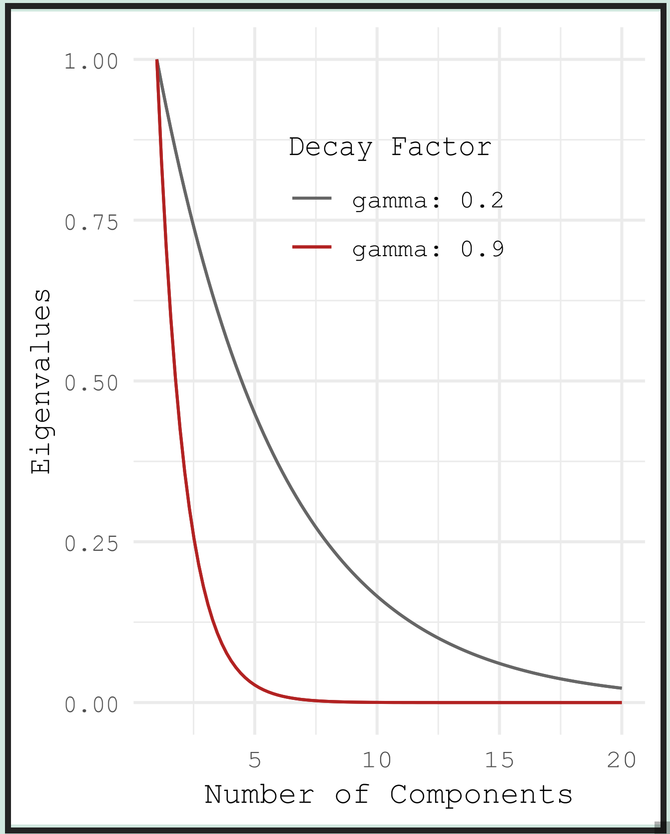
DESIGN OF THE COMPARISON EXPERIMENT

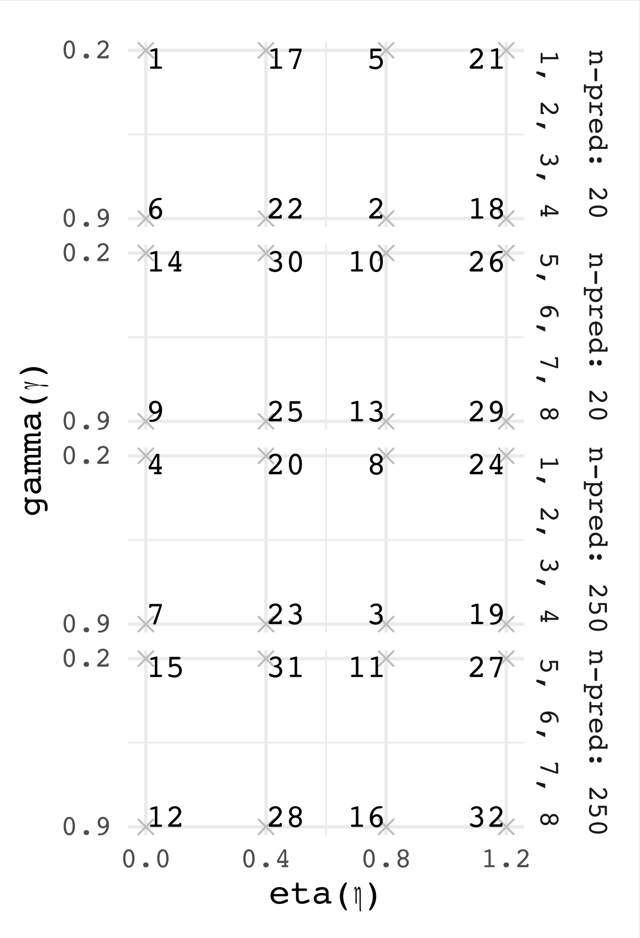
- High correlation between predictors
- High correlation between responses
- Relevant predictor components at position 5, 6, 7, 8

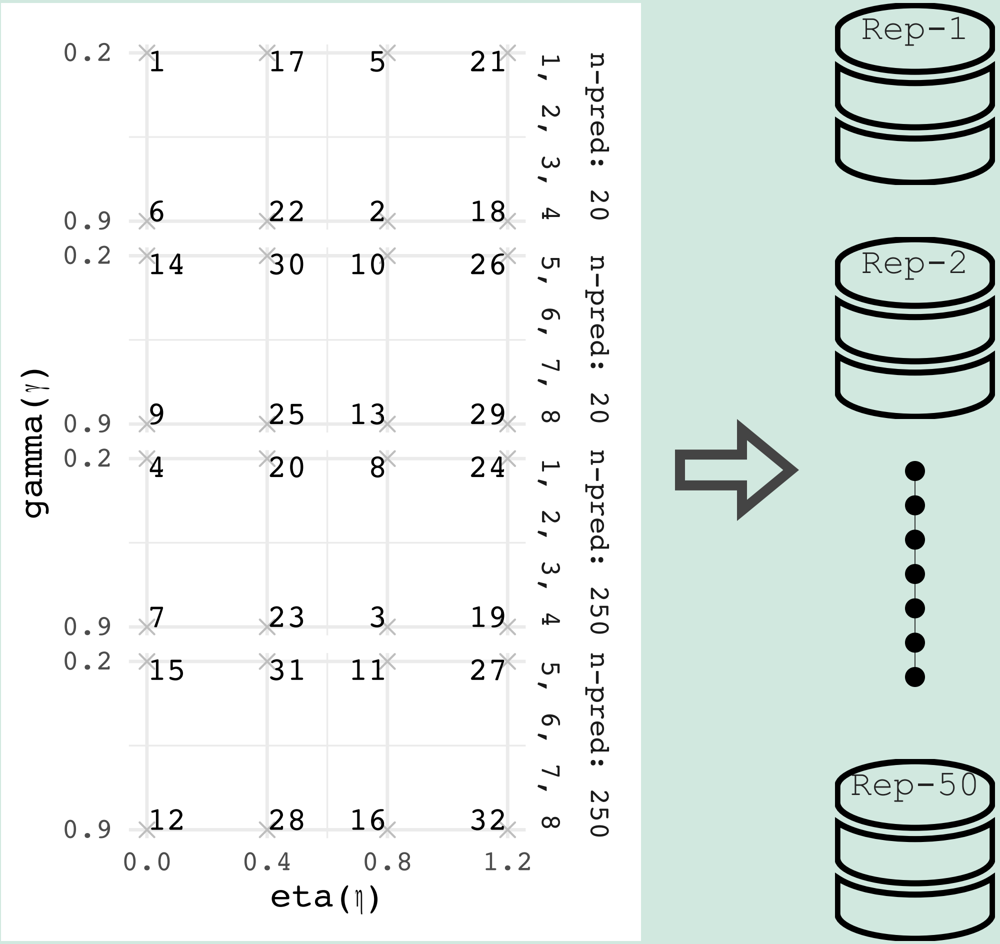
DESIGN 32

- Number of predictor variables: 250 $p > n$






gamma(γ)
eta(η)
0.2
0.9
0.0
0.4
0.8
1.2
n-pred: 20
n-pred: 250
1, 2, 3, 4
5, 6, 7, 8
1 17 5 21
6 22 2 18
14 30 10 26
9 25 13 29
4 20 8 24
7 23 3 19
15 31 11 27
12 28 16 32


0.2
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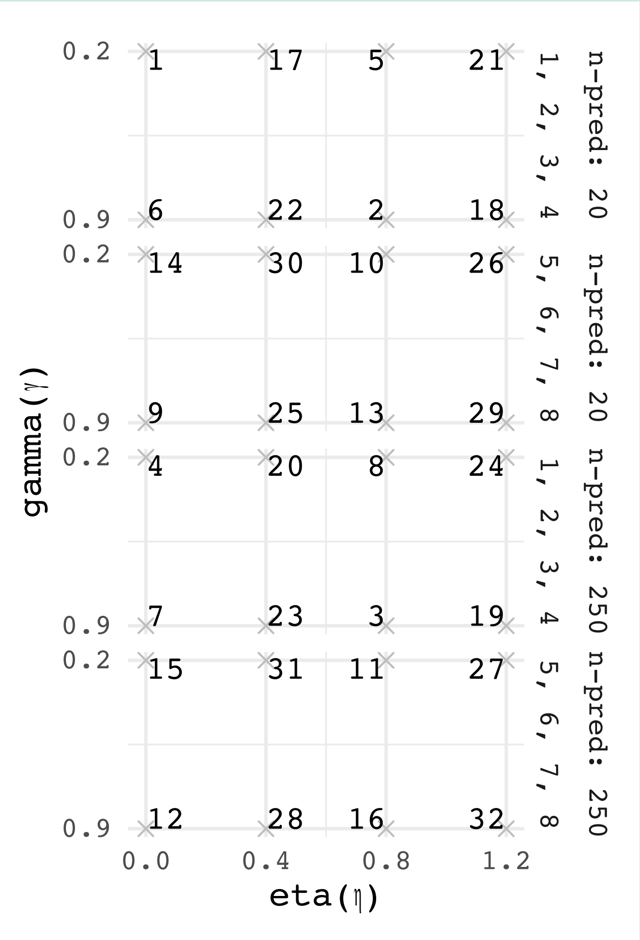
gamma(γ)
eta(η)
0.0
0.4
0.8
1.2
1 17 5 21
6 22 2 18
14 30 10 26
9 25 13 29
4 20 8 24
7 23 3 19
15 31 11 27
12 28 16 32
n-pred: 20
1, 2, 3, 4
n-pred: 20
5, 6, 7, 8
n-pred: 250
1, 2, 3, 4
n-pred: 250
5, 6, 7, 8
Rep-1
Rep-2
Rep-50


gamma(γ)
eta(η)
0.2
0.9
0.0
0.4
0.8
1.2
1
17
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29
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20
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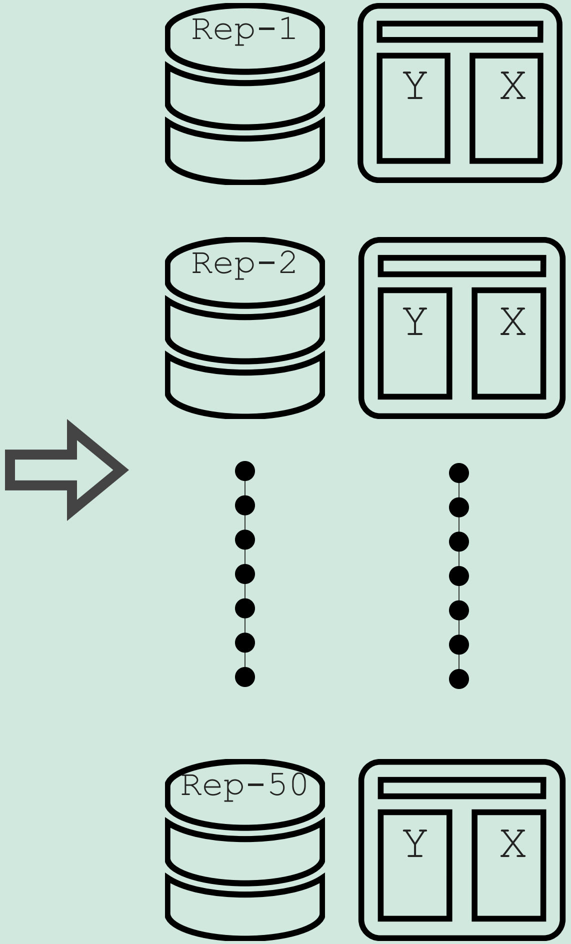
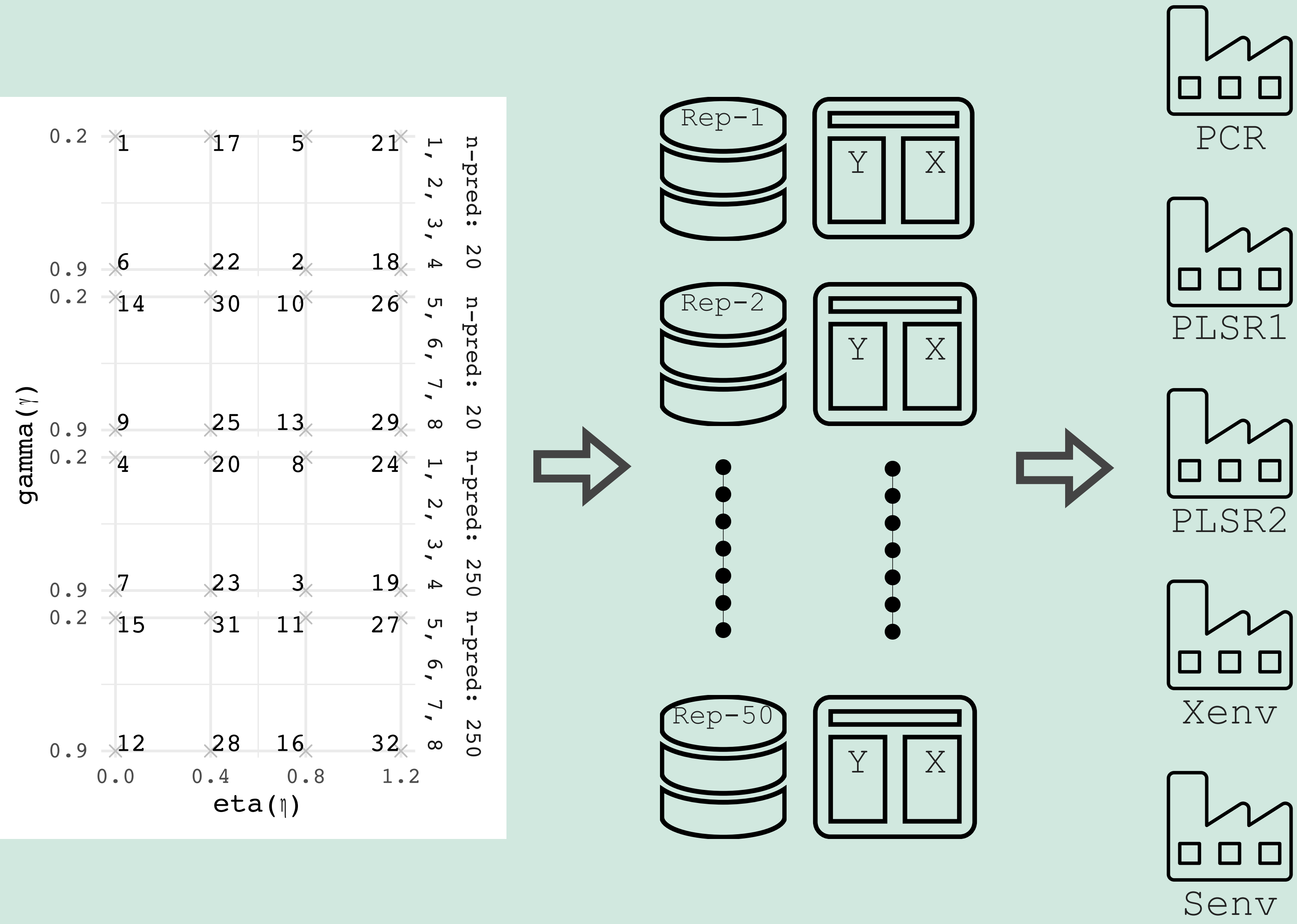
3
19
15
31
11
27
12
28
16
32
n-pred: 20
1, 2, 3, 4
n-pred: 20
5, 6, 7, 8
n-pred: 250
1, 2, 3, 4
n-pred: 250
5, 6, 7, 8


Rep-1
Y
X
Rep-2
Y
X
Rep-50
Y
X


0.2
0.9
0.2
0.9
0.2
0.9
0.2
0.9
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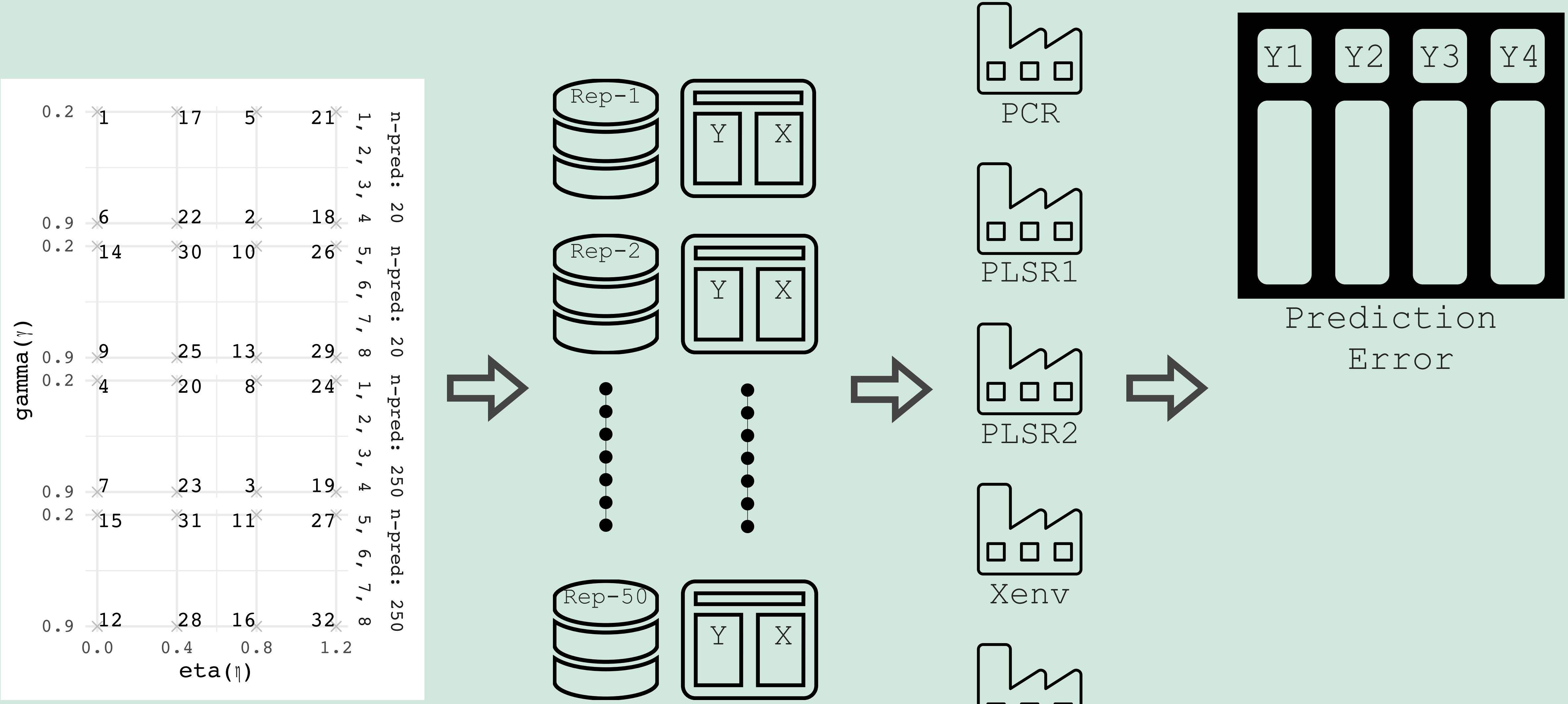
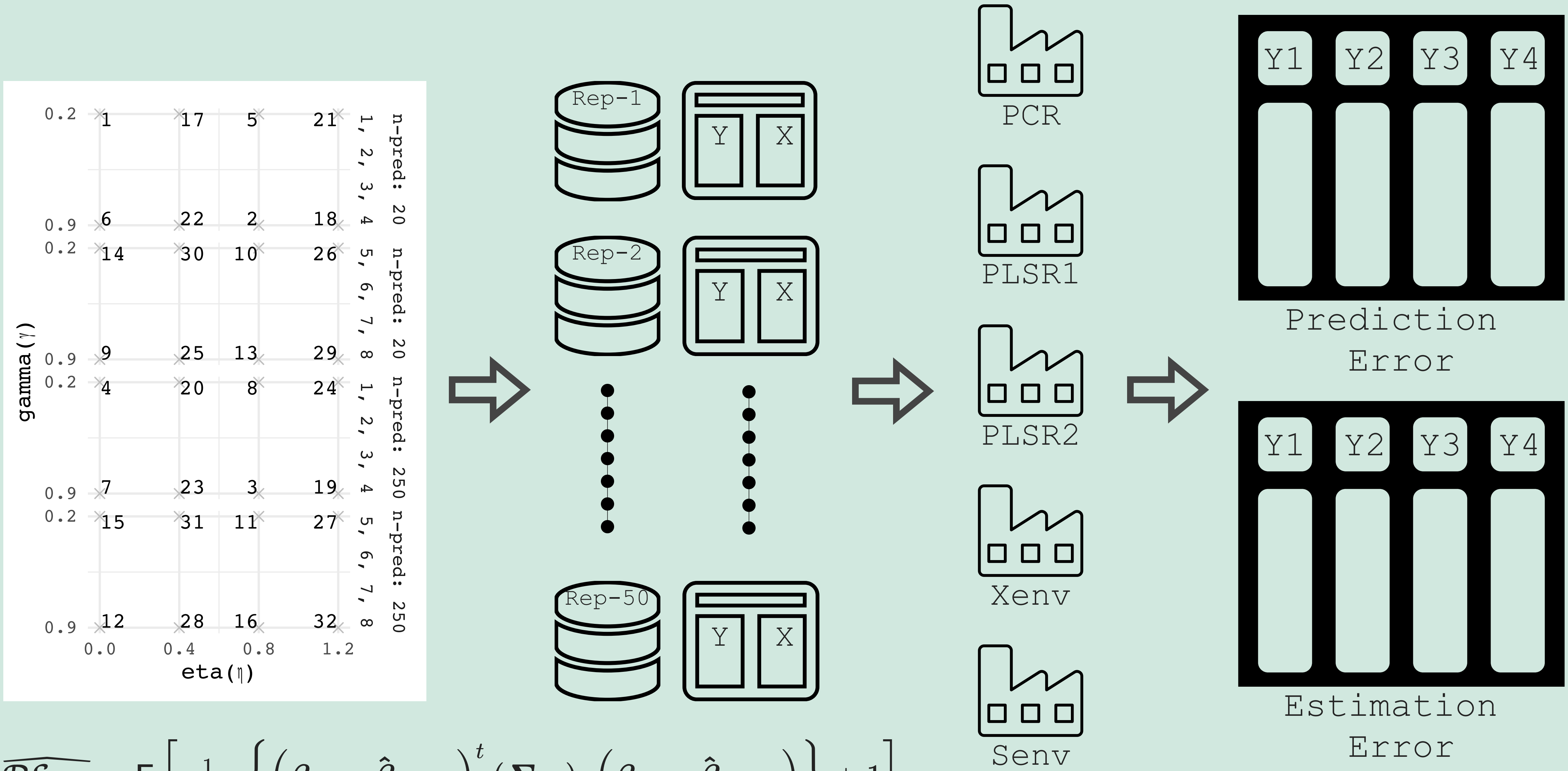
16
32
1, 2, 3, 4
n-pred: 20
5, 6, 7, 8
n-pred: 20
1, 2, 3, 4
n-pred: 250
5, 6, 7, 8
n-pred: 250
0.0
0.4
0.8
1.2
eta(η)
gamma(γ)
Rep-1
Y
X
Rep-2
Y
X
Rep-50
Y
X
PCR
PLSR1
PLSR2
Xenv
Senv



$$\widehat{\mathcal{PE}_{ijkl}} = \mathsf{E}\left[\frac{1}{\sigma^2_{y_{ij}|x}}\left\{\left(\boldsymbol{\beta}_{ij} - \hat{\boldsymbol{\beta}}_{\boldsymbol{ijklr}}\right)^t (\boldsymbol{\Sigma}_{xx})_i \left(\boldsymbol{\beta}_{ij} - \hat{\boldsymbol{\beta}}_{\boldsymbol{ijklr}}\right)\right\} + 1\right]$$



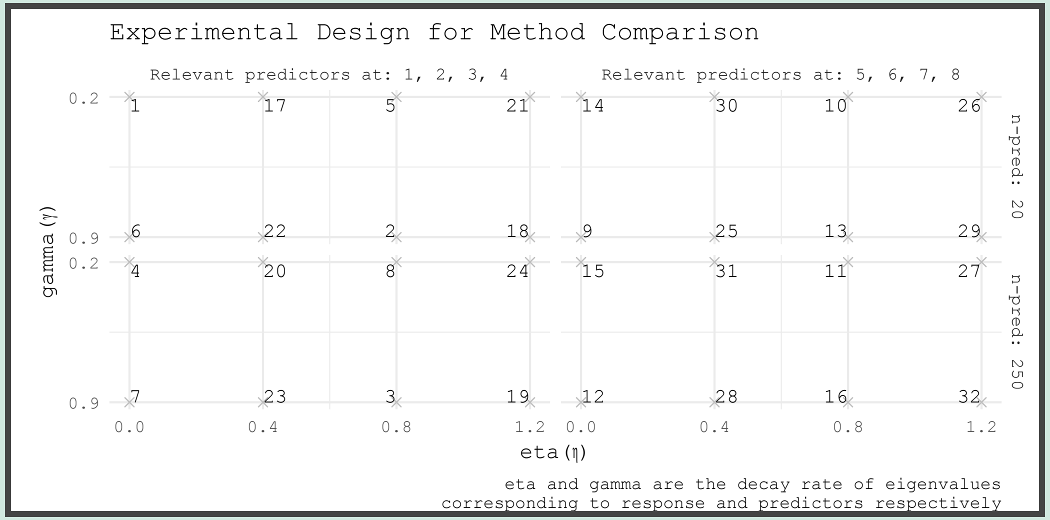
$$\widehat{\mathcal{PE}}_{ijkl} = \mathsf{E}\left[\frac{1}{\sigma^2_{y_{ij}|x}}\left\{\left(\boldsymbol{\beta}_{ij} - \hat{\boldsymbol{\beta}}_{\boldsymbol{ijklr}}\right)^t (\boldsymbol{\Sigma}_{xx})_i \left(\boldsymbol{\beta}_{ij} - \hat{\boldsymbol{\beta}}_{\boldsymbol{ijklr}}\right)\right\} + 1\right]$$

$$\mathrm{MSE}\left(\widehat{\boldsymbol{\beta}}\right)_{ijkl} = \mathsf{E}\left[\frac{1}{\sigma^2_{y_j}}\left(\boldsymbol{\beta}_{ij} - \widehat{\boldsymbol{\beta}}_{\boldsymbol{ijkl}}\right)^t\left(\boldsymbol{\beta}_{ij} - \widehat{\boldsymbol{\beta}}_{\boldsymbol{ijkl}}\right)\right]$$

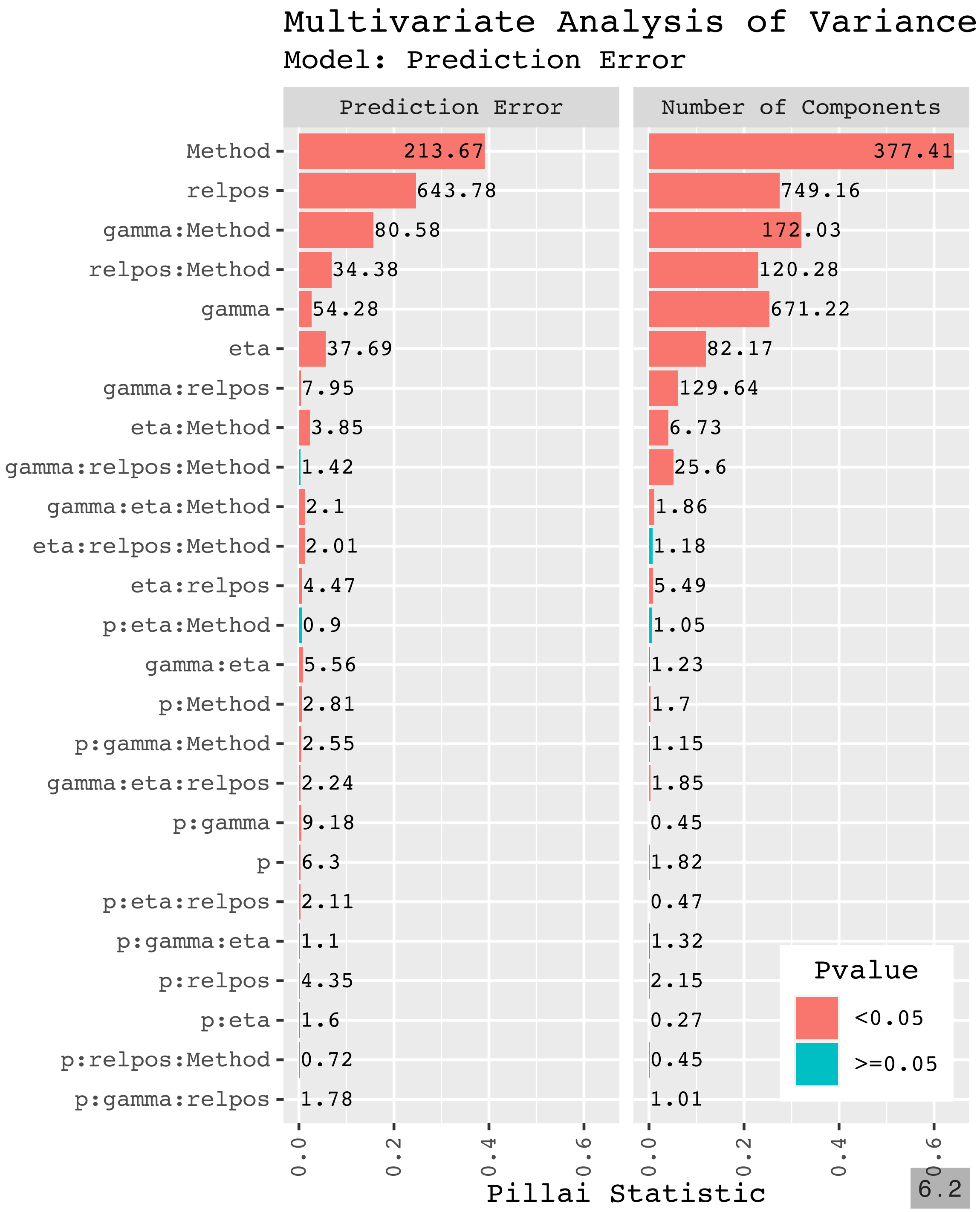
COMPARISON OF MULTI-RESPONSE MULTIVARIATE METHODS

PREDICTION & ESTIMATION ERROR

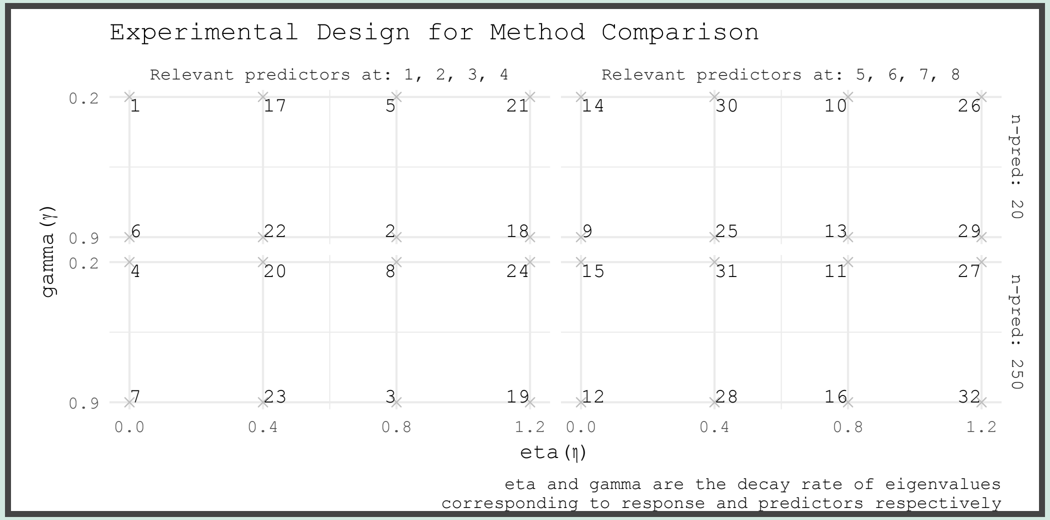
PREDICTION COMPARISON




```
# A tibble: 88,000 x 11
      p     relpos      eta   gamma Method    Y1    Y2    Y3    Y4
    <fct> <fct>        <fct> <fct> <chr>  <dbl> <dbl> <dbl> <dbl>
  1 20    1, 2, 3, 4 0       0.2   PCR     1.01  1.16  1.07  2.35
  2 20    1, 2, 3, 4 0       0.2   PLSR1   1.62  1.02  1.57  1.03
  3 20    1, 2, 3, 4 0       0.2   PLSR2   1.70  1.04  1.13  1.32
  4 20    1, 2, 3, 4 0       0.2   Senv    2.16  1.17  1.00  1.13
  5 20    1, 2, 3, 4 0       0.2   Xenv    1.24  1.01  1.04  2.26
  6 250   5, 6, 7, 8 1.2     0.9   PCR     1.70  2.04  2.46  3.02
  7 250   5, 6, 7, 8 1.2     0.9   PLSR1   1.80  2.53  2.22  2.66
  8 250   5, 6, 7, 8 1.2     0.9   PLSR2   1.34  1.07  3.28  4.10
  9 250   5, 6, 7, 8 1.2     0.9   Senv    2.28  4.68  1.14  1.24
 10 250   5, 6, 7, 8 1.2     0.9   Xenv    2.00  1.15  3.33  2.75
# … with 87,990 more rows
```

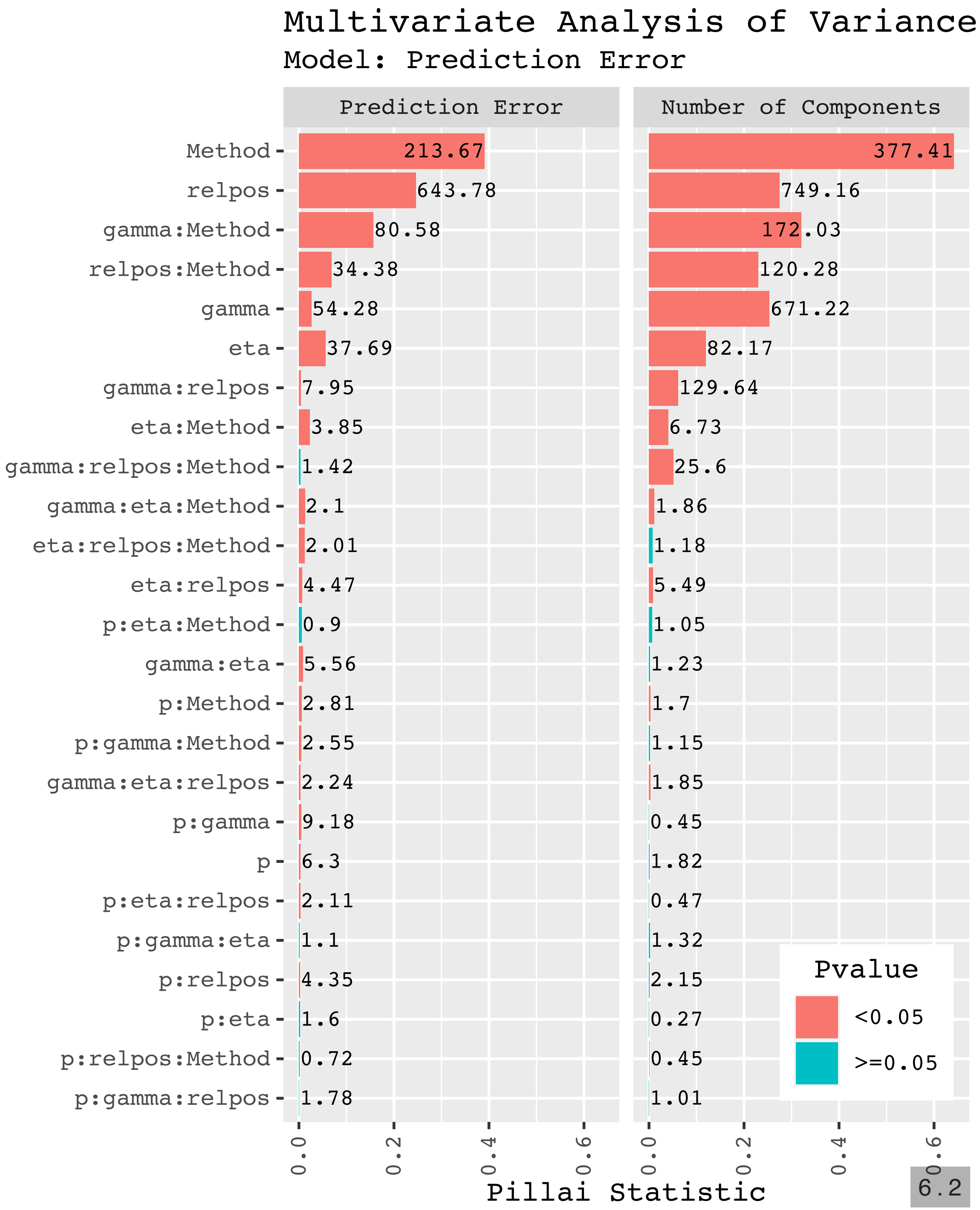


PREDICTION COMPARISON

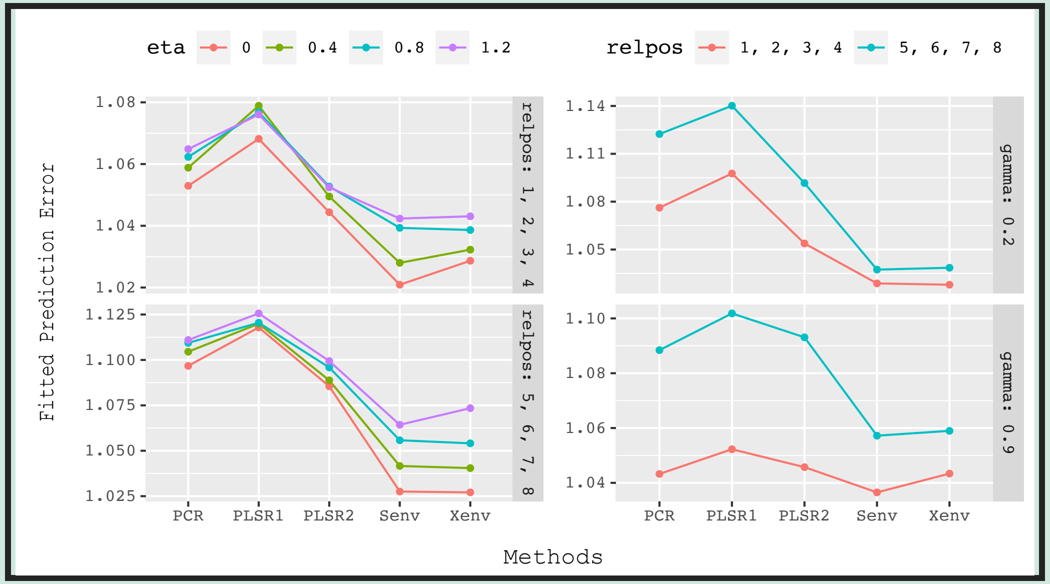


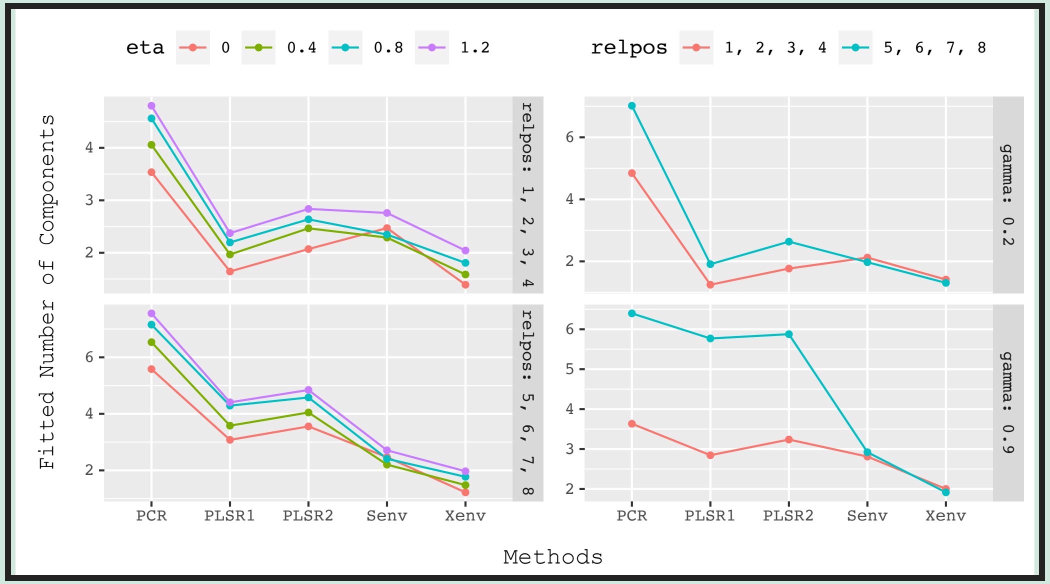

```
# A tibble: 88,000 x 11
      p     relpos      eta    gamma Method     Y1     Y2     Y3     Y4
    <fct> <fct>        <fct> <fct> <chr>   <dbl>  <dbl>  <dbl>  <dbl>
  1 20     1, 2, 3, 4 0      0.2   PCR      1.01   1.16   1.07   2.35
  2 20     1, 2, 3, 4 0      0.2   PLSR1    1.62   1.02   1.57   1.03
  3 20     1, 2, 3, 4 0      0.2   PLSR2    1.70   1.04   1.13   1.32
  4 20     1, 2, 3, 4 0      0.2   Senv     2.16   1.17   1.00   1.13
  5 20     1, 2, 3, 4 0      0.2   Xenv     1.24   1.01   1.04   2.26
  6 250    5, 6, 7, 8 1.2    0.9   PCR      1.70   2.04   2.46   3.02
  7 250    5, 6, 7, 8 1.2    0.9   PLSR1    1.80   2.53   2.22   2.66
  8 250    5, 6, 7, 8 1.2    0.9   PLSR2    1.34   1.07   3.28   4.10
  9 250    5, 6, 7, 8 1.2    0.9   Senv     2.28   4.68   1.14   1.24
 10 250    5, 6, 7, 8 1.2    0.9   Xenv     2.00   1.15   3.33   2.75
# … with 87,990 more rows
```

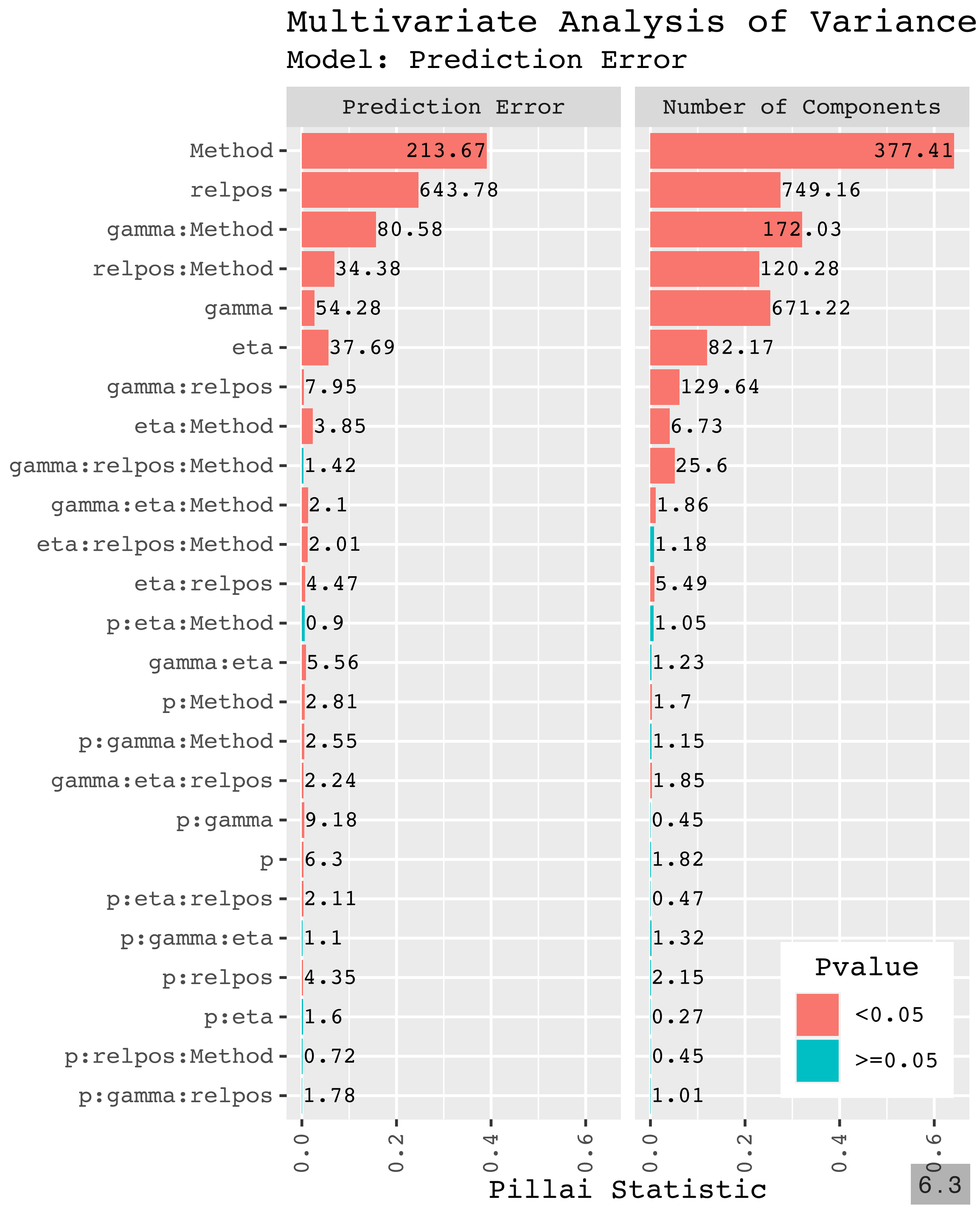
```
cbind(Y1, Y2, Y3, Y4) ~
  (p + gamma + eta + relpos + Method)^3
```



PREDICTION COMPARISON

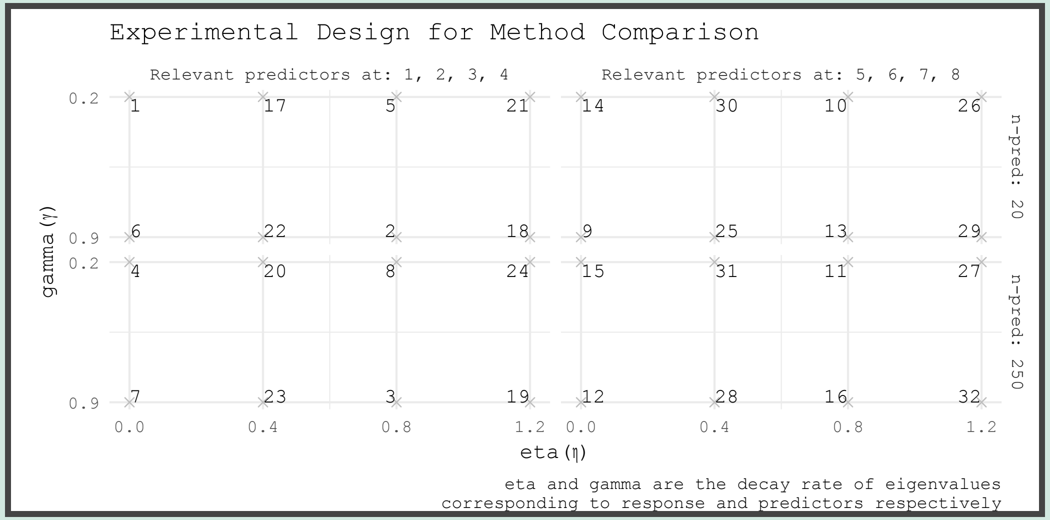




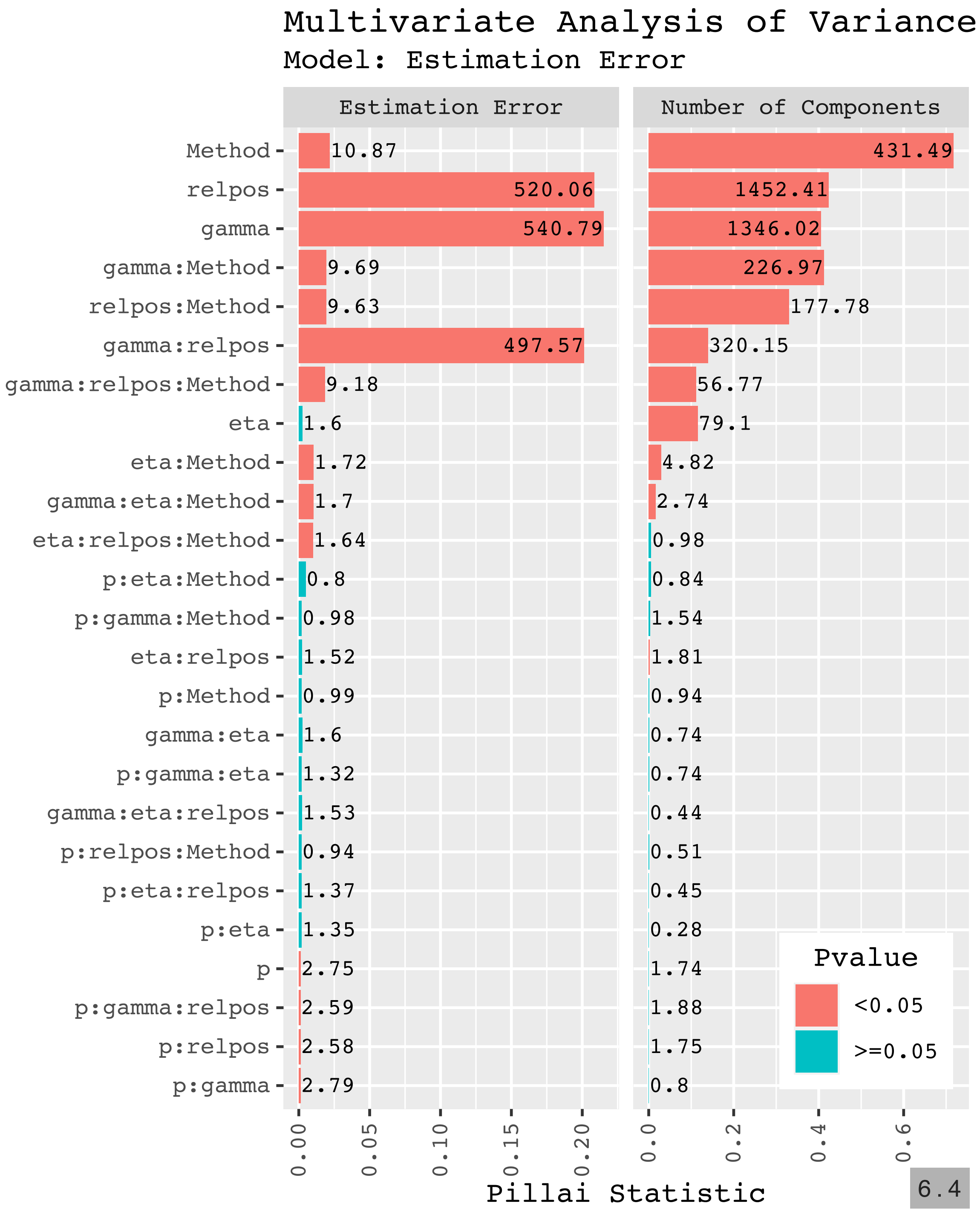


6.3

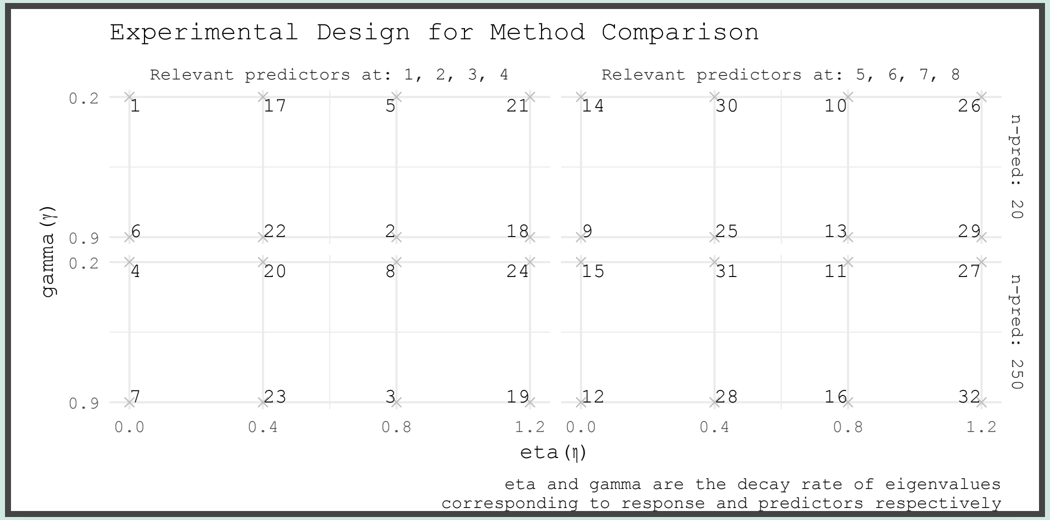
ESTIMATION COMPARISON




```
# A tibble: 88,000 x 9
      p     relpos      eta   gamma Method        Y1        Y2         Y3        Y
  <fct> <fct>        <fct> <fct> <chr>      <dbl>     <dbl>      <dbl>     <db
 1 20    1, 2, 3, 4 0     0.2   PCR       0.0210    0.209     0.103       0.85
 2 20    1, 2, 3, 4 0     0.2   PLSR1     0.535     0.0338    0.507       0.04
 3 20    1, 2, 3, 4 0     0.2   PLSR2     0.598     0.0492    0.162       0.35
 4 20    1, 2, 3, 4 0     0.2   Senv      0.748     0.202     0.000139    0.16
 5 20    1, 2, 3, 4 0     0.2   Xenv      0.242     0.0182    0.0423      0.69
 6 250   5, 6, 7, 8 1.2   0.9   PCR     113.      140.      164.        184.
 7 250   5, 6, 7, 8 1.2   0.9   PLSR1    87.8     119.      108.        123.
 8 250   5, 6, 7, 8 1.2   0.9   PLSR2    75.9      18.2     206.        224.
 9 250   5, 6, 7, 8 1.2   0.9   Senv    140.      197.       31.5        48.3
10 250   5, 6, 7, 8 1.2   0.9   Xenv     96.3      24.5     135.        122.
# … with 87,990 more rows
```

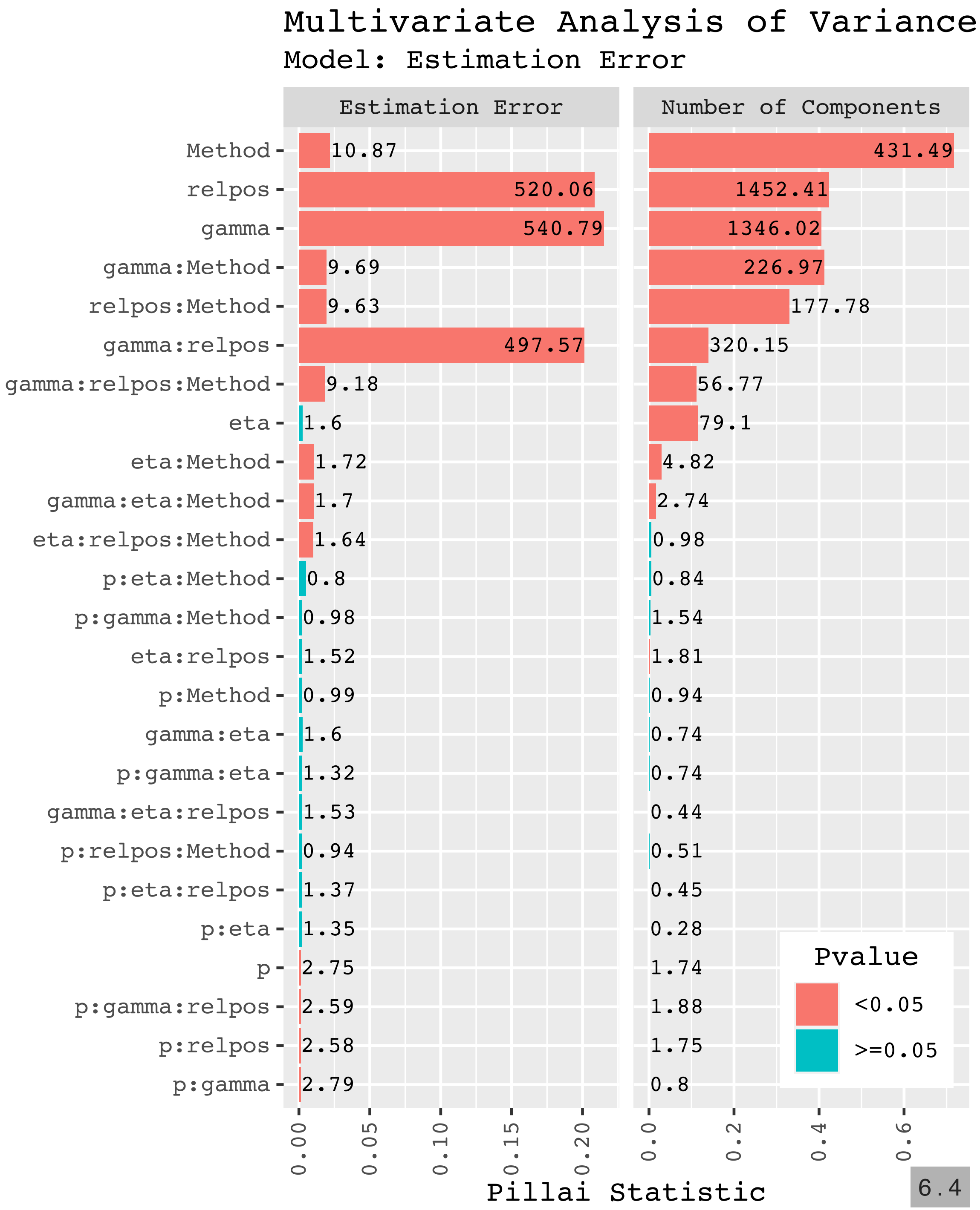


ESTIMATION COMPARISON

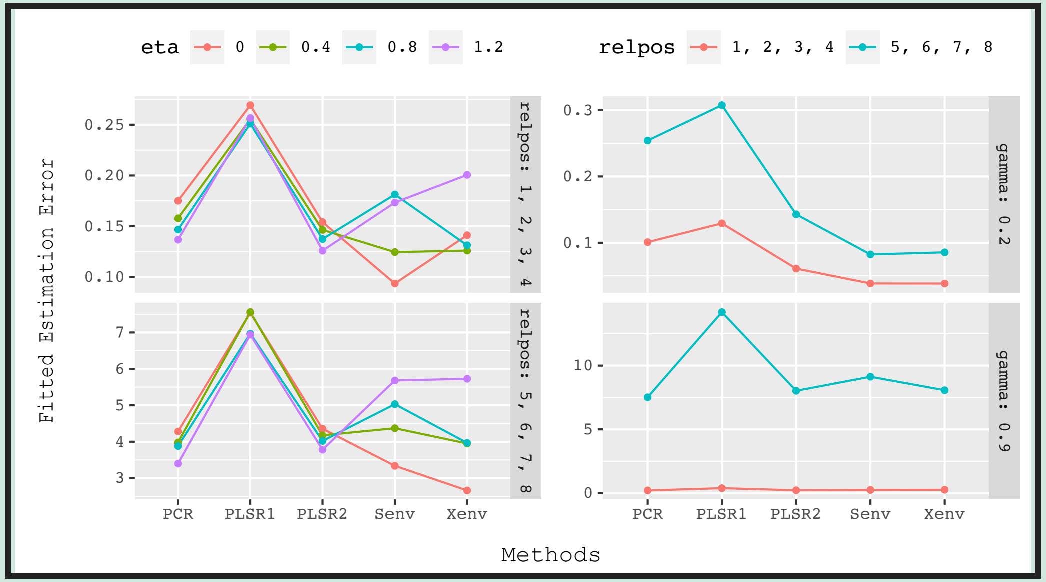


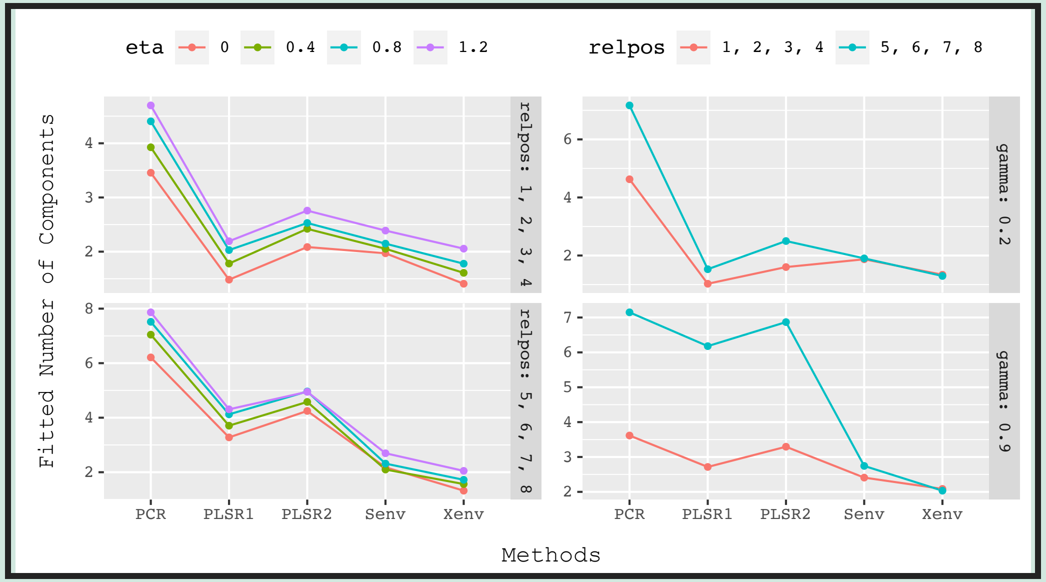

```
# A tibble: 88,000 x 9
      p  relpos      eta   gamma Method        Y1       Y2         Y3       Y
  <fct> <fct>      <fct> <fct> <chr>      <dbl>    <dbl>      <dbl>    <db
  1 20   1, 2, 3, 4 0    0.2   PCR       0.0210   0.209     0.103     0.85
  2 20   1, 2, 3, 4 0    0.2   PLSR1     0.535    0.0338    0.507     0.04
  3 20   1, 2, 3, 4 0    0.2   PLSR2     0.598    0.0492    0.162     0.35
  4 20   1, 2, 3, 4 0    0.2   Senv      0.748    0.202     0.000139  0.16
  5 20   1, 2, 3, 4 0    0.2   Xenv      0.242    0.0182    0.0423    0.69
  6 250  5, 6, 7, 8 1.2  0.9   PCR     113.     140.      164.      184.
  7 250  5, 6, 7, 8 1.2  0.9   PLSR1    87.8    119.      108.      123.
  8 250  5, 6, 7, 8 1.2  0.9   PLSR2    75.9     18.2     206.      224.
  9 250  5, 6, 7, 8 1.2  0.9   Senv    140.     197.       31.5      48.3
 10 250  5, 6, 7, 8 1.2  0.9   Xenv     96.3     24.5     135.      122.
# … with 87,990 more rows
```

```
cbind(Y1, Y2, Y3, Y4) ~
  (p + gamma + eta + relpos + Method)^3
```



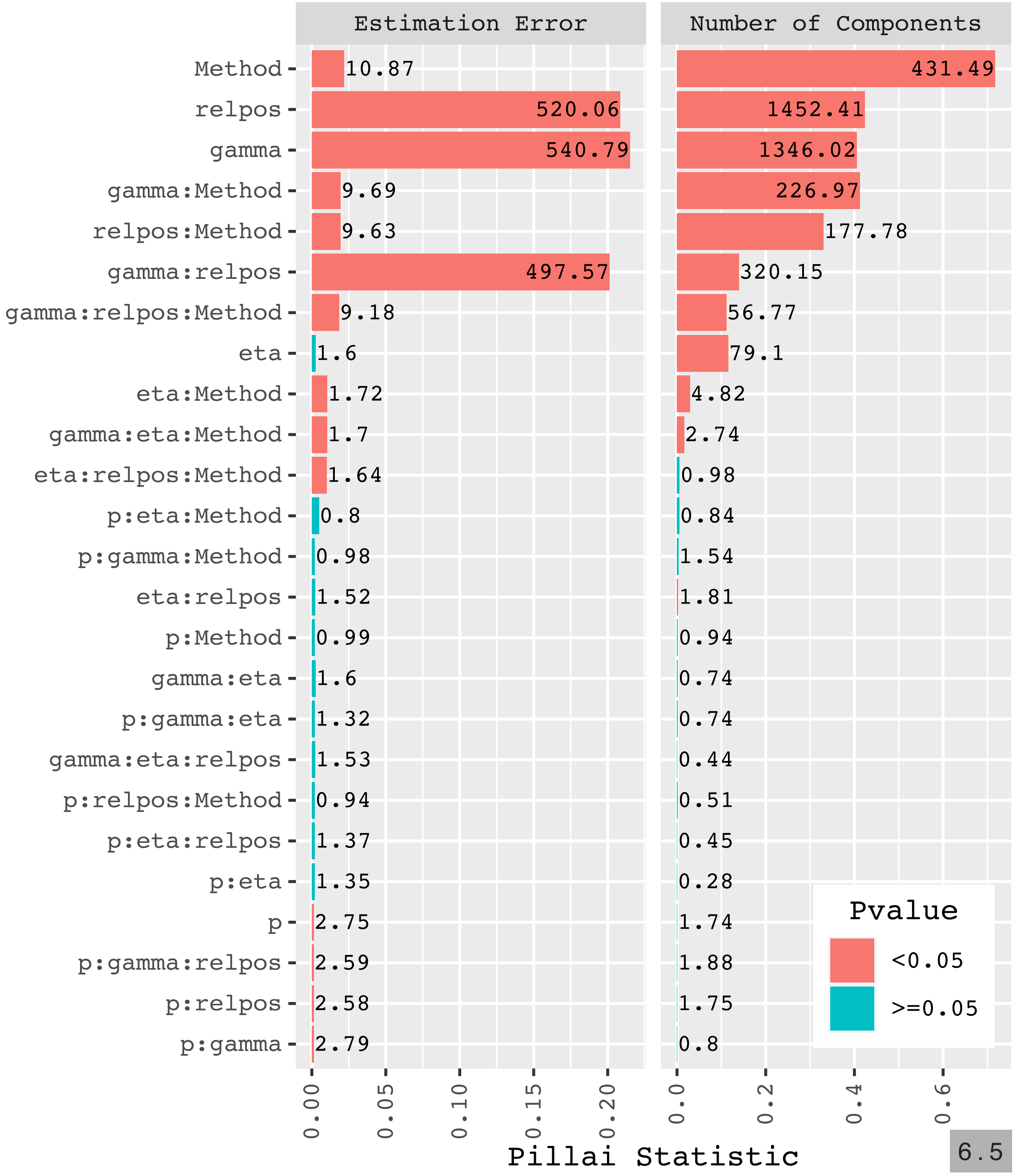
ESTIMATION COMPARISON





Multivariate Analysis of Variance

Model: Estimation Error



CONCLUDING REMARKS

ACHIEVEMENTS, REPRODUCIBILITY, LIMITATIONS & PROSPECTS

ACHIEVEMENTS

- *Added a toolbox* to the scientific community that is also applicable for academic purpose
- Provided an *extensive comparative study* of the multi-response model with new and established methods
- Can become *reference literature* for researchers where they can identify methods for their use based on the properties of their data

REPRODUCIBILITY

- All the study and research papers are *open-access* and the codes are *open-source*
- To reproduce the study, codes are available on *GitHub* with detail instructions
- Docker *containers* and analysis *code* together with the *text* of the research article give complete *control* for the reproduction

`https://github.com/therimalaya/thesis`

LIMITATIONS

- Assumptions in the simrel tool
- Categorical Response and Categorical Predictors
- Have not included shrinkage based methods like Ridge, Lasso and Elastic Net
- Machine learning algorithms could have been included

PERSPECTS

- The assumptions can be removed in order to make the simulation more robust and flexible
- Extend the use of the tool in education together with research
- Non-normal distribution/ ANOVA Model/ Categorical Responses
- A tool that can suggest the simulation parameters based on the data

ACKNOWLEDGMENT

SUPERVISORS

SOLVE SÆBØ

TRYGVE ALMØY

BioStatistics

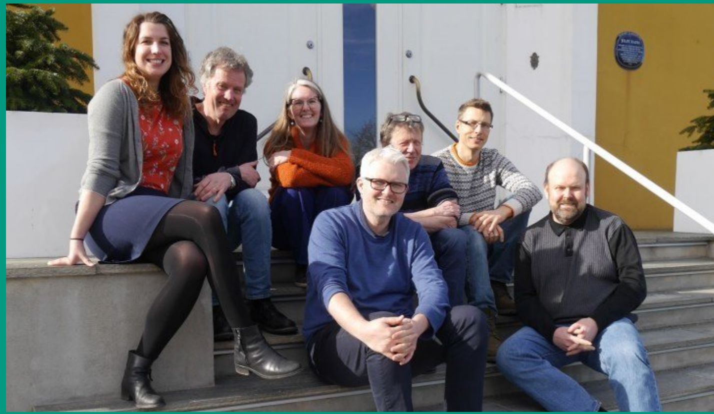
Norges miljø- og biovitenskapelige universitet

ACKNOWLEDGMENT

SUPERVISORS

SOLVE SÆBØ

TRYGVE ALMØY



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Yes! I enjoyed
the journey.


Dakujem
TAK
teşekkür ederim
salamat
hvala
mersi
HVALA
감사합니다
Ευχαριστω
kiitos
merc
GRAZZii
salama
GRAZAS
TAKK
Рахмет
MAHALO
arigato
takk
ARiGATO
Thank You
suwun
MERCi
teşekkür ederim
DANKE
kiitos
hvala
mahalo
GRAZAS
ありかとっ
SUWUN
TAKK
多謝
спасибо
gracias

THANK YOU

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