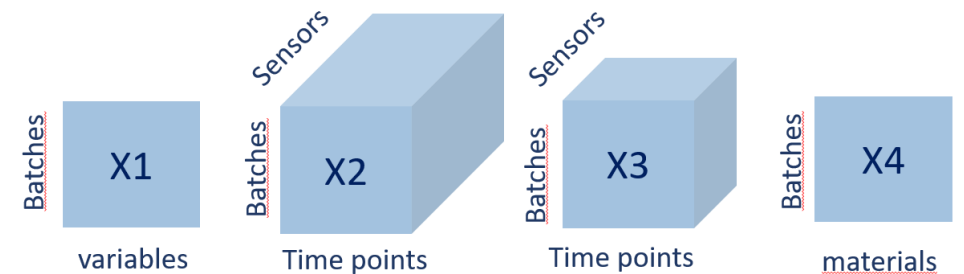
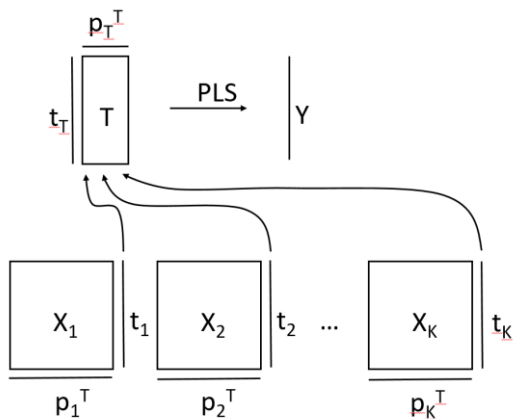


(Multiblock) PLS for Python chemometrics for a new audience?

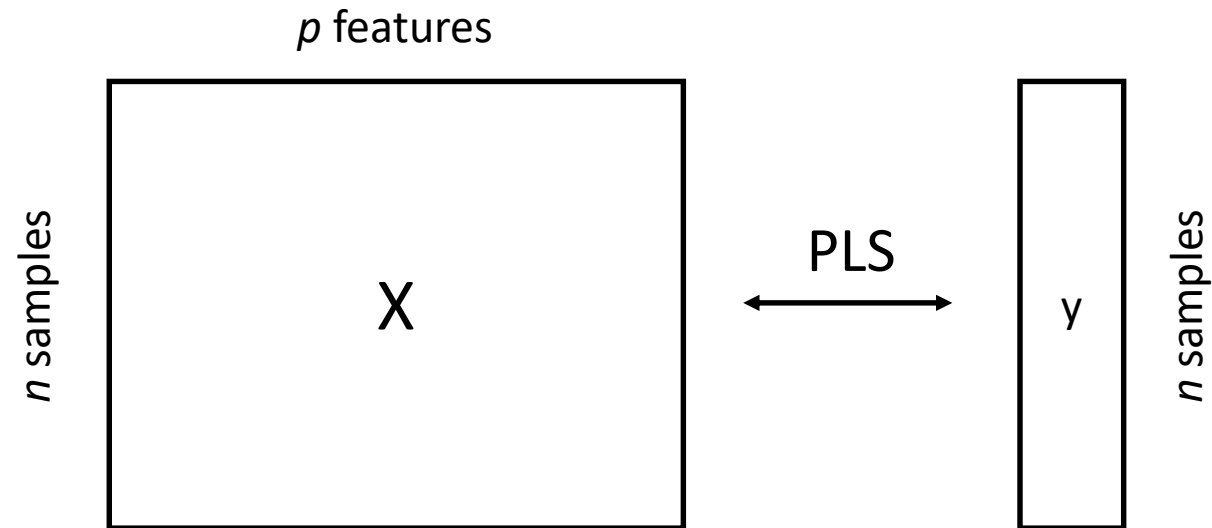
Andreas Baum, Laurent Vermue

andba@dtu.dk

Department of Applied Mathematics and Computer Science, Technical University of Denmark

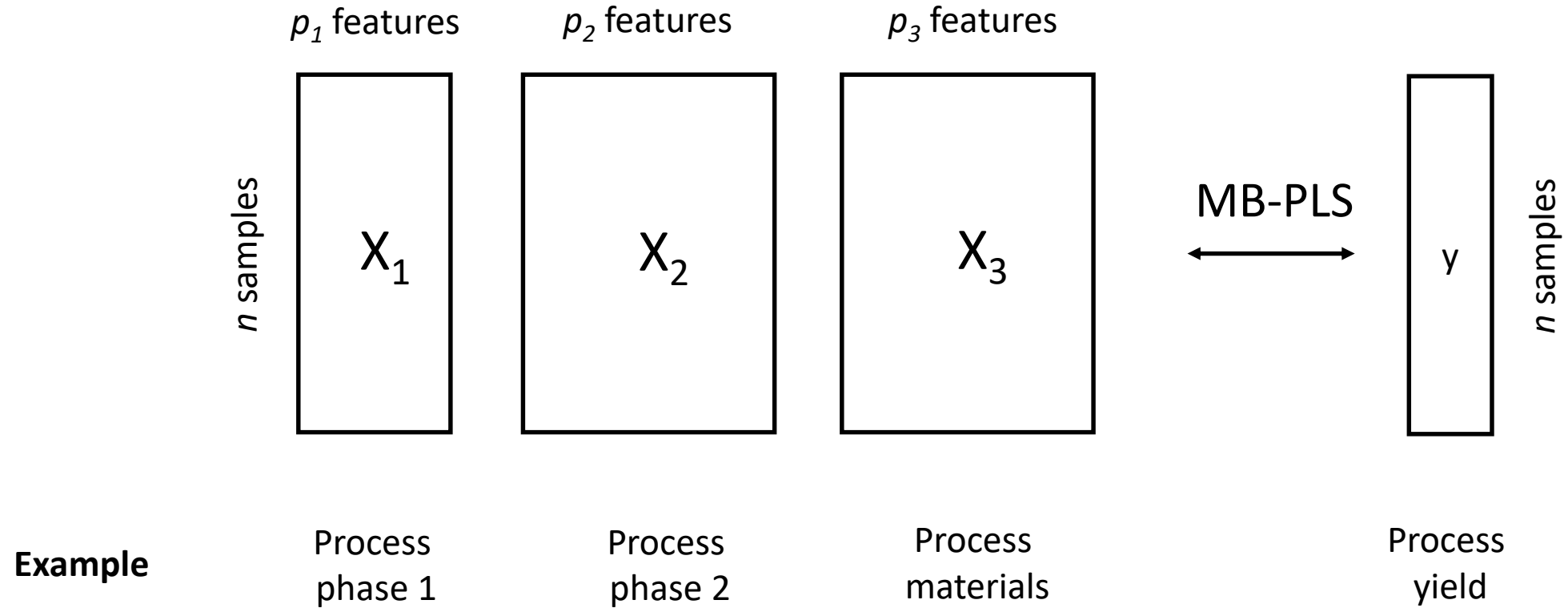


Partial Least Squares (PLS)

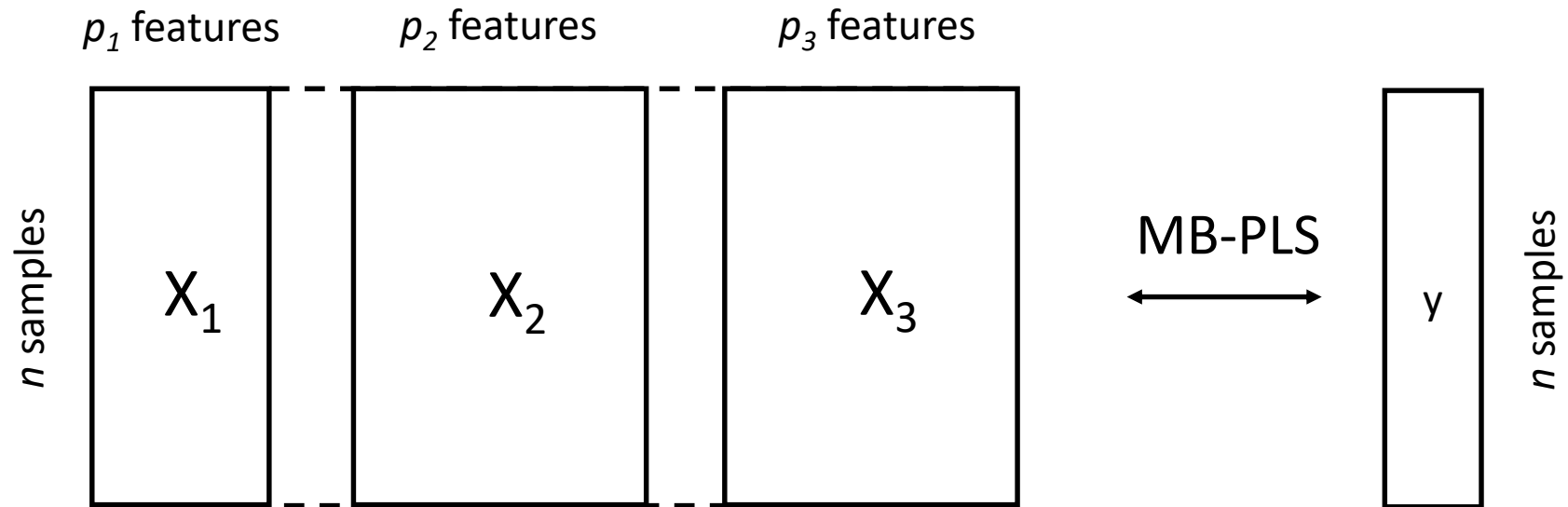


- PLS good when:
- many features
 - features are cross-correlated (e.g. spectroscopic data)

Why MB-PLS?



Why MB-PLS?



Example

Process
phase 1

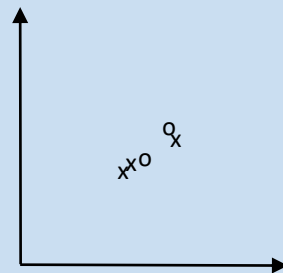
Process
phase 2

Process
materials

Process
yield

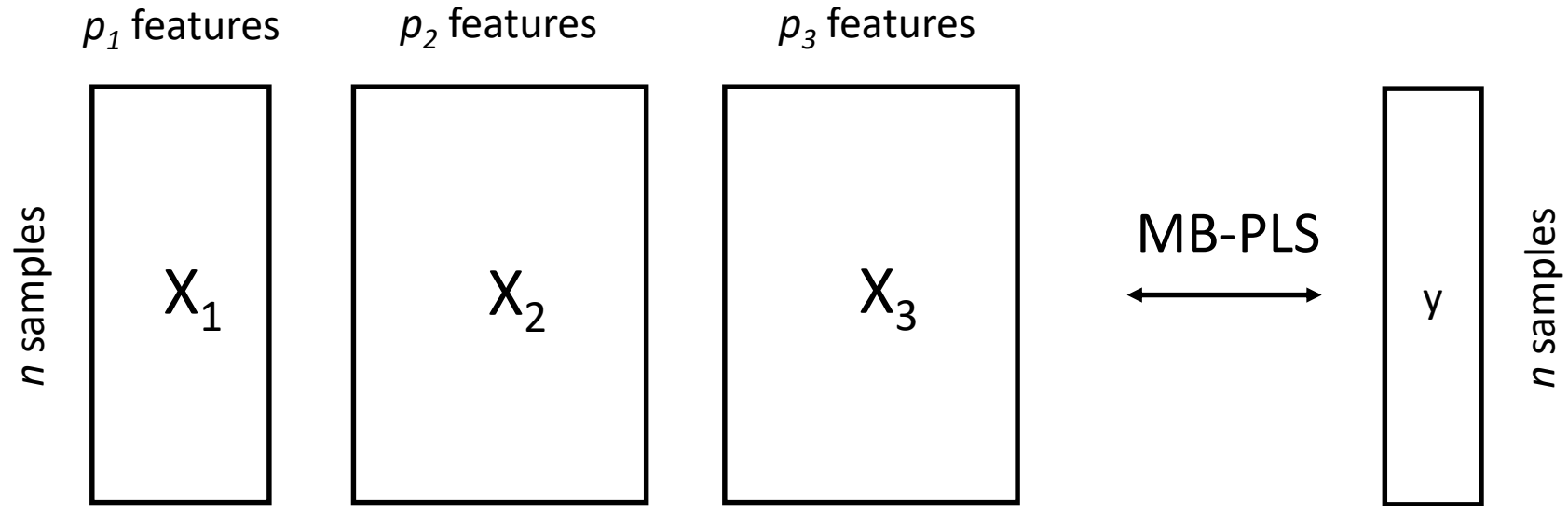
PLS

Latent Variables
Exploratory Analysis



65% explained
variance

Why MB-PLS?



Example

Process
phase 1

Process
phase 2

Process
materials

Process
yield

MB-PLS

**Block
Importance**

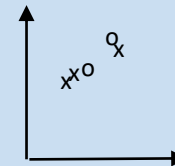
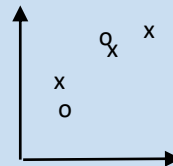
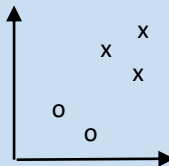
35%

15%

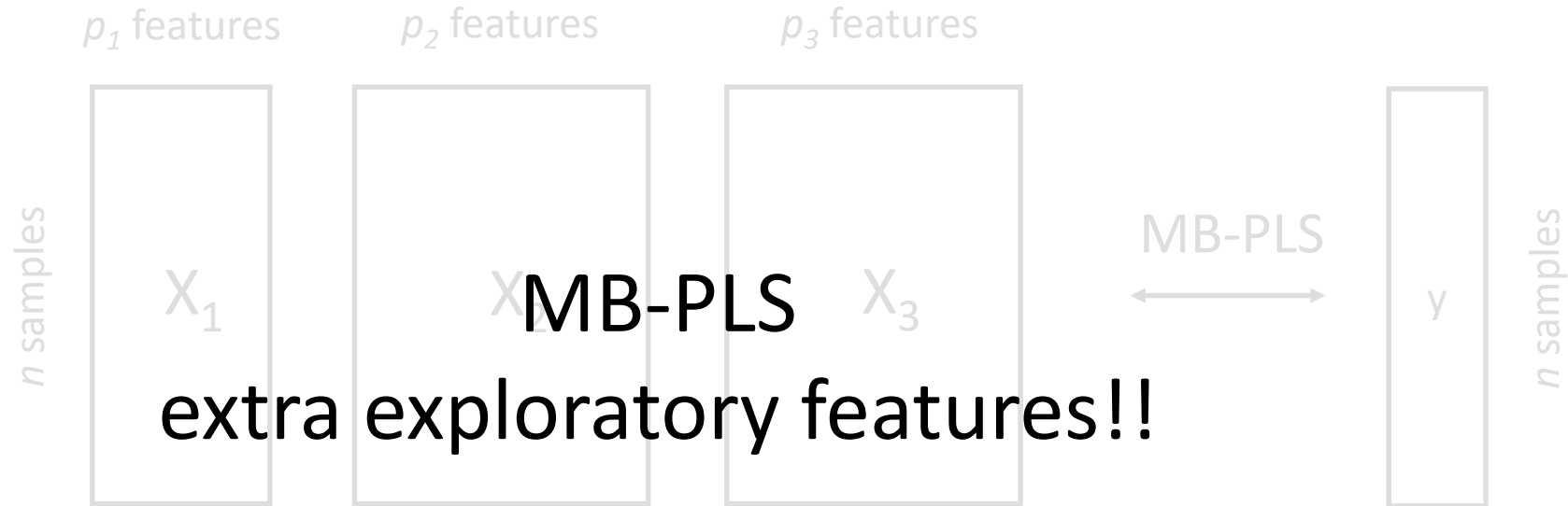
50%

65% explained
variance

**Latent Variables
Exploratory Analysis**



Why MB-PLS?



example

Process
phase 1

Process
phase 2

Process
materials

Process
yield

MB-PLS

**Block
Importance**

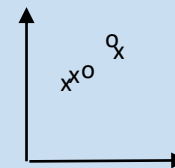
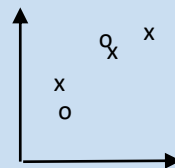
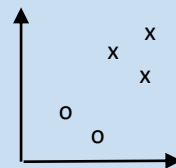
35%

15%

50%

65% explained
variance

**Latent Variables
Exploratory Analysis**



Open Source Software?

R

MB-PLS
Ade4 for modeling of
ecological data

Python

OnPLS
modeling of
orthogonal and shared
components

Matlab

SO-PLS, PO-PLS

Open Source Software?

R

MB-PLS
Ade4 for modeling of
ecological data

Python

OnPLS
modeling of
orthogonal and shared
components

Matlab

SO-PLS, PO-PLS

(MB)-PLS Package for Python

- Open source: <https://github.com/b0nsaii/MBPLS>
- Easy to install and use (includes Quickstart)
- Can handle missing data
- Build upon Scikit Learn API and model selection toolbox (including Preprocessing, CV, Pipelines, GridSearch etc)
- Github hosted: contributors are welcome 😊
- It is FAST! Algorithms improved, benchmark tests performed

b0nsaii / MBPLS

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(Multiblock) Partial Least Squares regression for python

Edit

Manage topics

92 commits 3 branches 0 releases 2 contributors BSD-3-Clause

Branch: Package_OOP New pull request Create new file Upload files Find file Clone or download

b0nsaii	modify README.md	Latest commit 8c68b67 a minute ago
examples	modify README.md	an hour ago
mbpls	Fix array transformation error with NIPALS method	a day ago
.gitignore	Implemented add_noise method	2 months ago
LICENSE.txt	Add BSD-license to package	9 days ago
README.md	modify README.md	a minute ago
pytest.ini	- Enabled testing via pytest	2 months ago
setup.py	Fix bug concerning one block non-standardized models and version update	2 days ago

README.md

Partial Least Squares Package

An easy to use Python package for (Multiblock) Partial Least Squares prediction modelling of univariate or multivariate outcomes. Four state of the art algorithms have been implemented and optimized for robust performance on large data matrices. The package has been designed to be able to handle missing data, such that application is straight forward using the commonly known Scikit-Learn API and its model selection toolbox.

Installation

- Install the package for Python3 using the following command. Some dependencies might require an upgrade (scikit-learn, numpy and scipy).

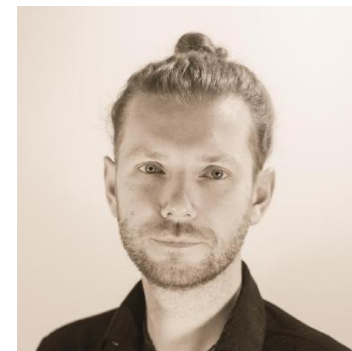
```
$ pip install mbpls
```

Contributors

Laurent Vermue



Andreas Baum



Check it out!

github.com/b0nsaii/MBPLS