A FRAMEWORK FOR BILINEAR CALIBRATION TRANSFER BASED ON TRANSFER LEVELS

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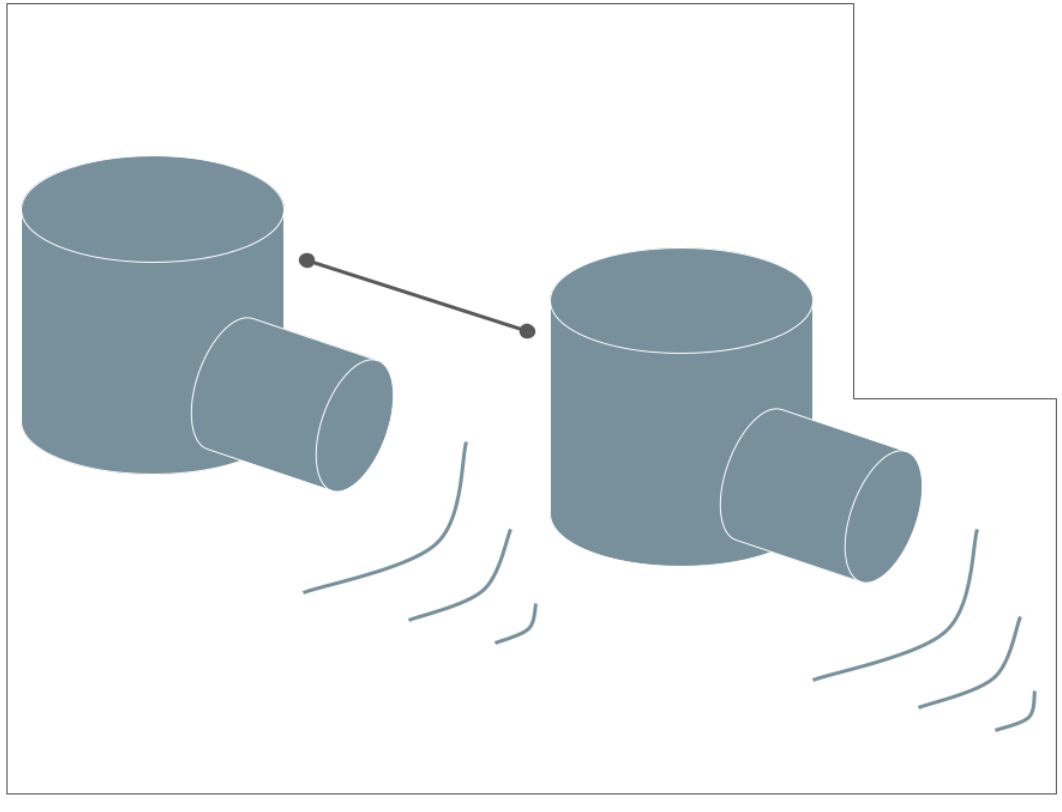
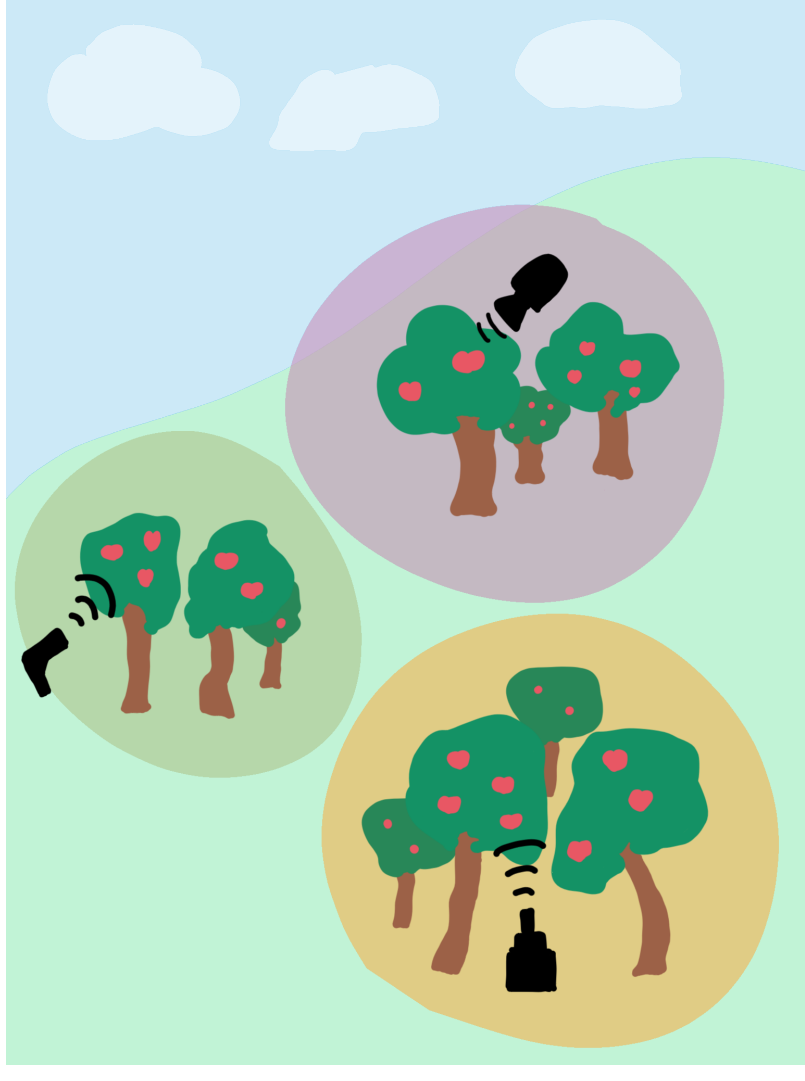
Classical instrument standardization



Modern calibration transfer

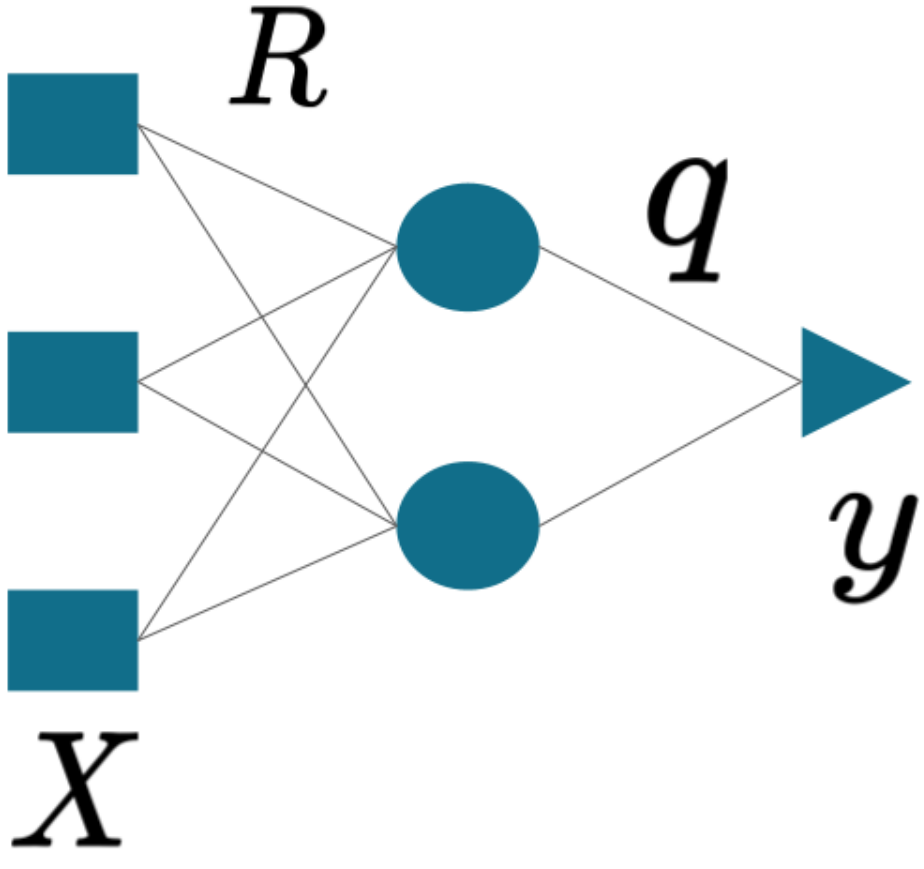


CALIBRATION TRANSFER

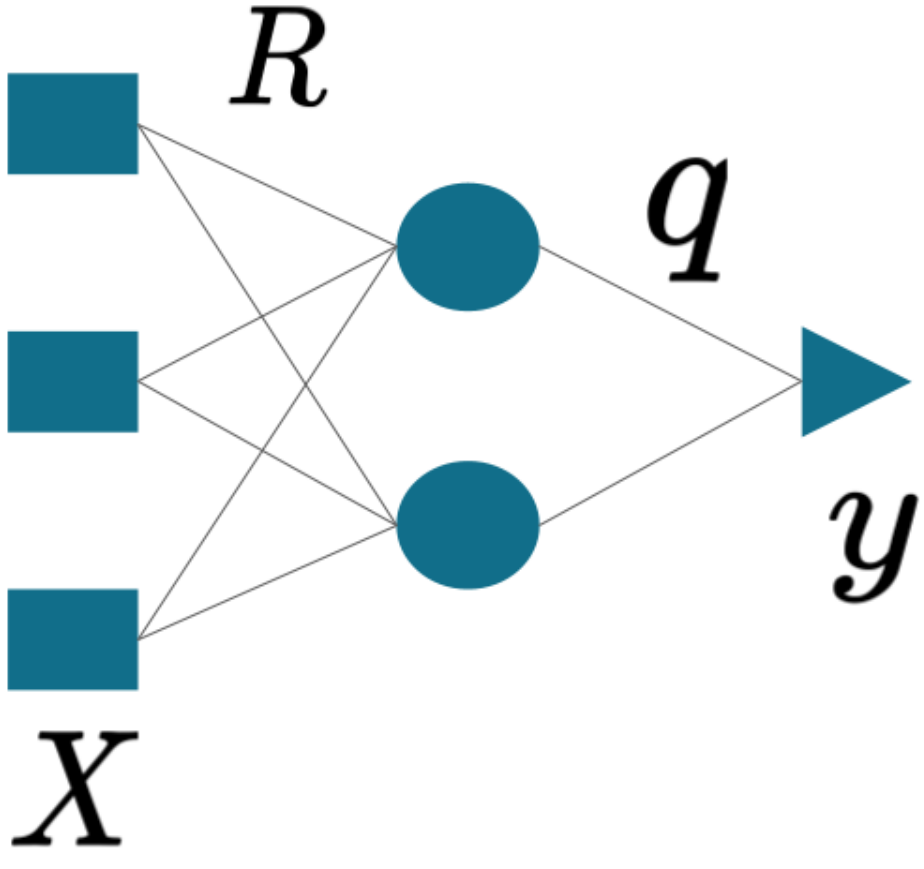
Motivated by transfer learning *(Pan, S. et al. 2010)*

Calibration transfer may refer to retain and reuse a previous calibration model and adapting it for a new domain (typically an instrument).

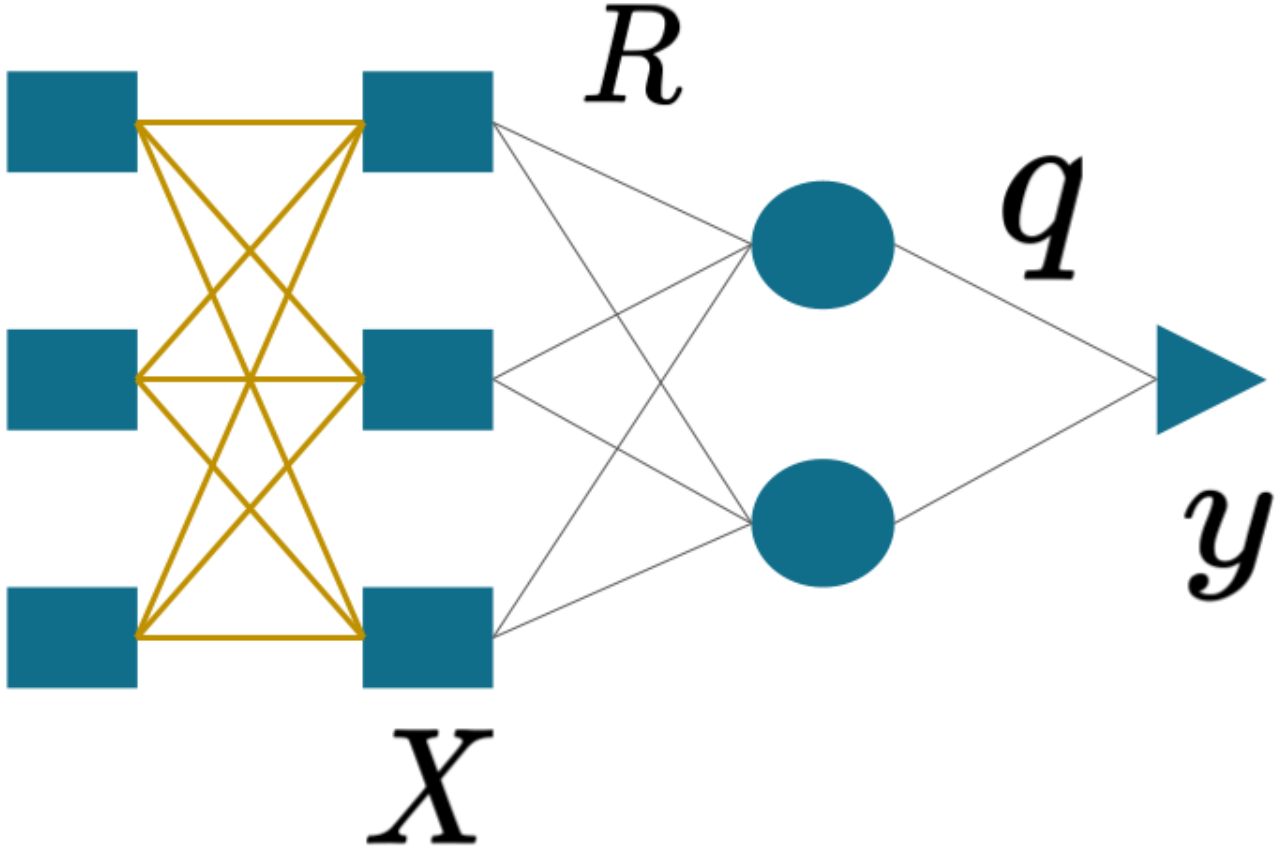
Bilinear models: Interpretation of the calibration model *(Naes, T. et al. 2004)*



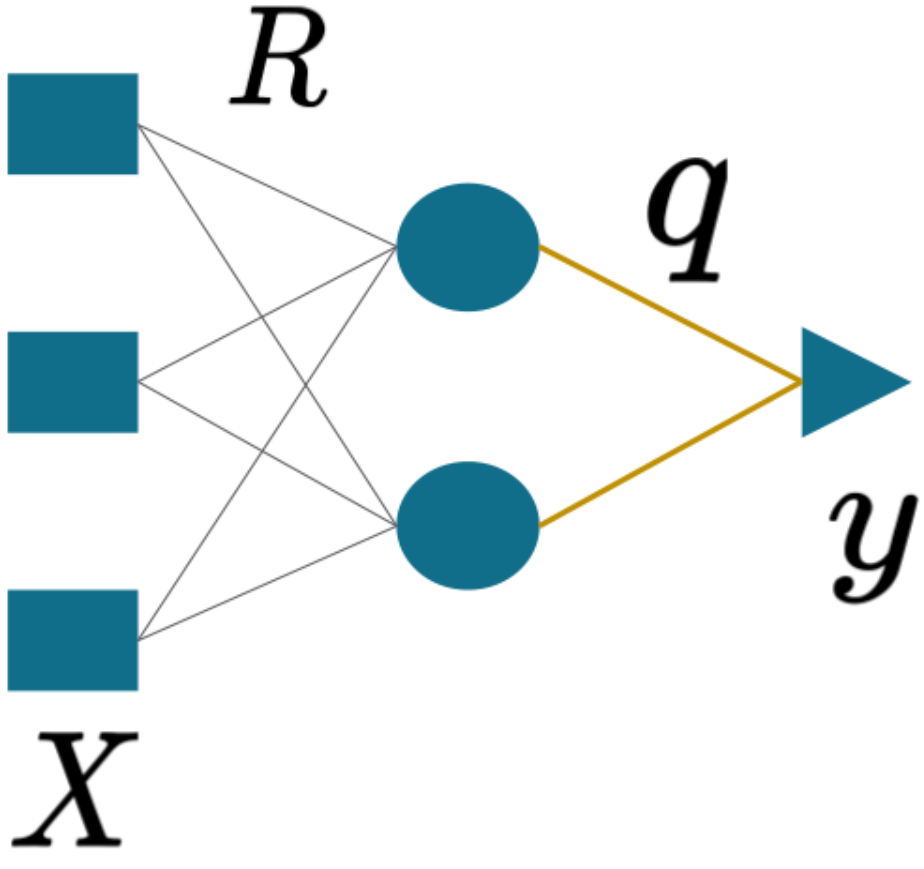
Framework: Calibration transfer can occur at different levels



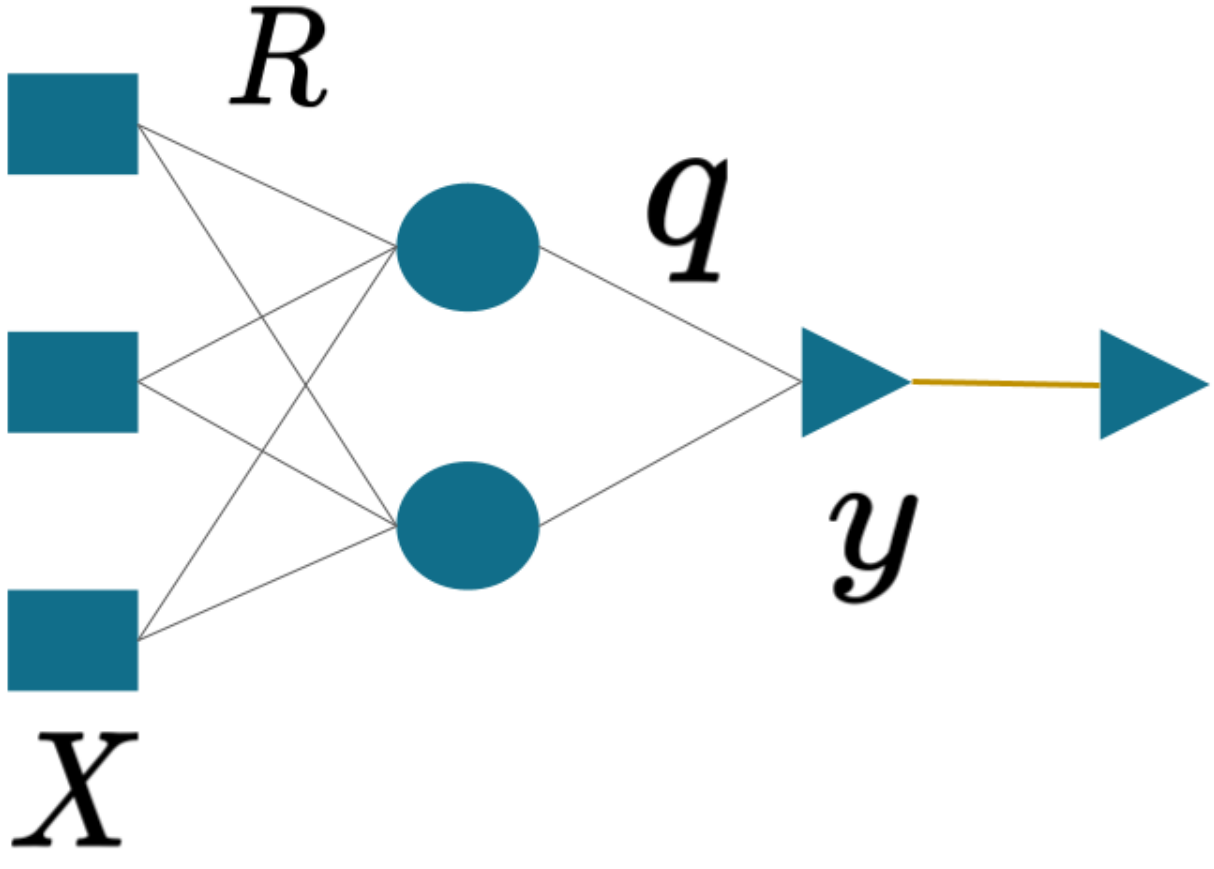
Instrument transfer level: (Piecewise) Direct Standardization *(Wang, Y. et al. 1991)*, Orthogonalization *(Zeaiter, M. et al. 2006. Roger, JM. et al. 2003)*



Xy **transfer level:** Joint Y PLS *(Garcia, S. et al. 2005)*



Xy **transfer level:** Slope and Bias Correction *(Fearn, T. et al. 2001)*



Recalibration using Domain Invariant PLS *(Nikzad-Langerodi, R. et al. 2018)*

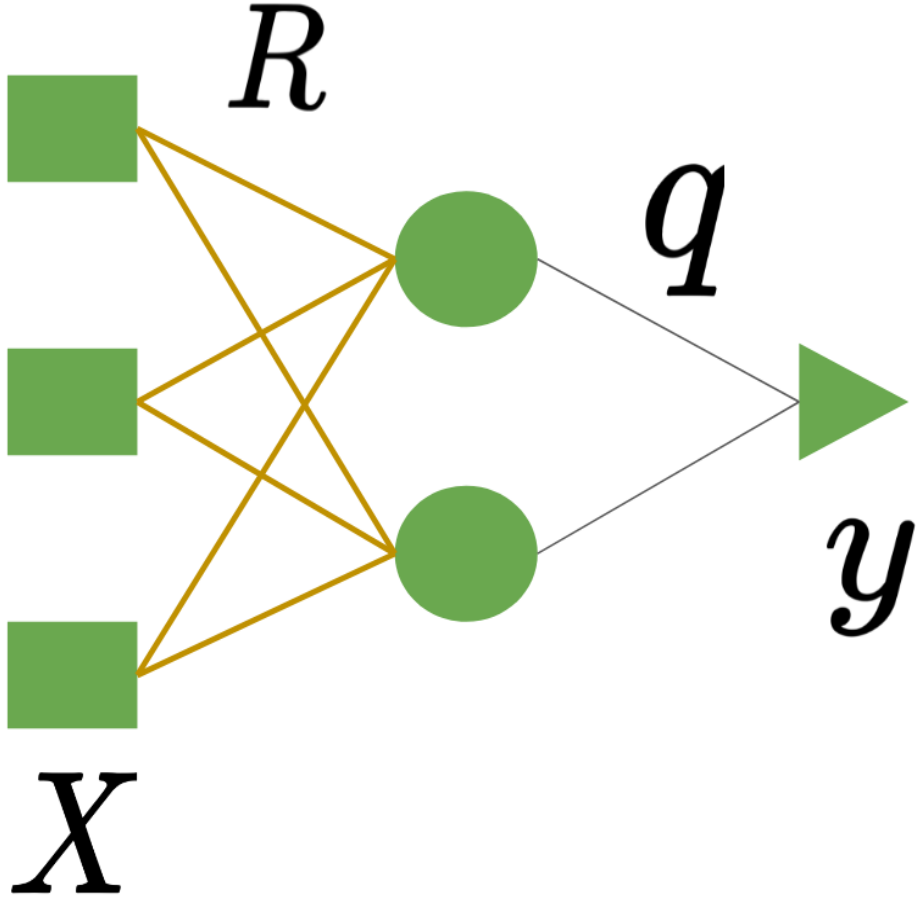
Xy transfer level

$$\min_{w} ||X - yw^T||$$

subject to:

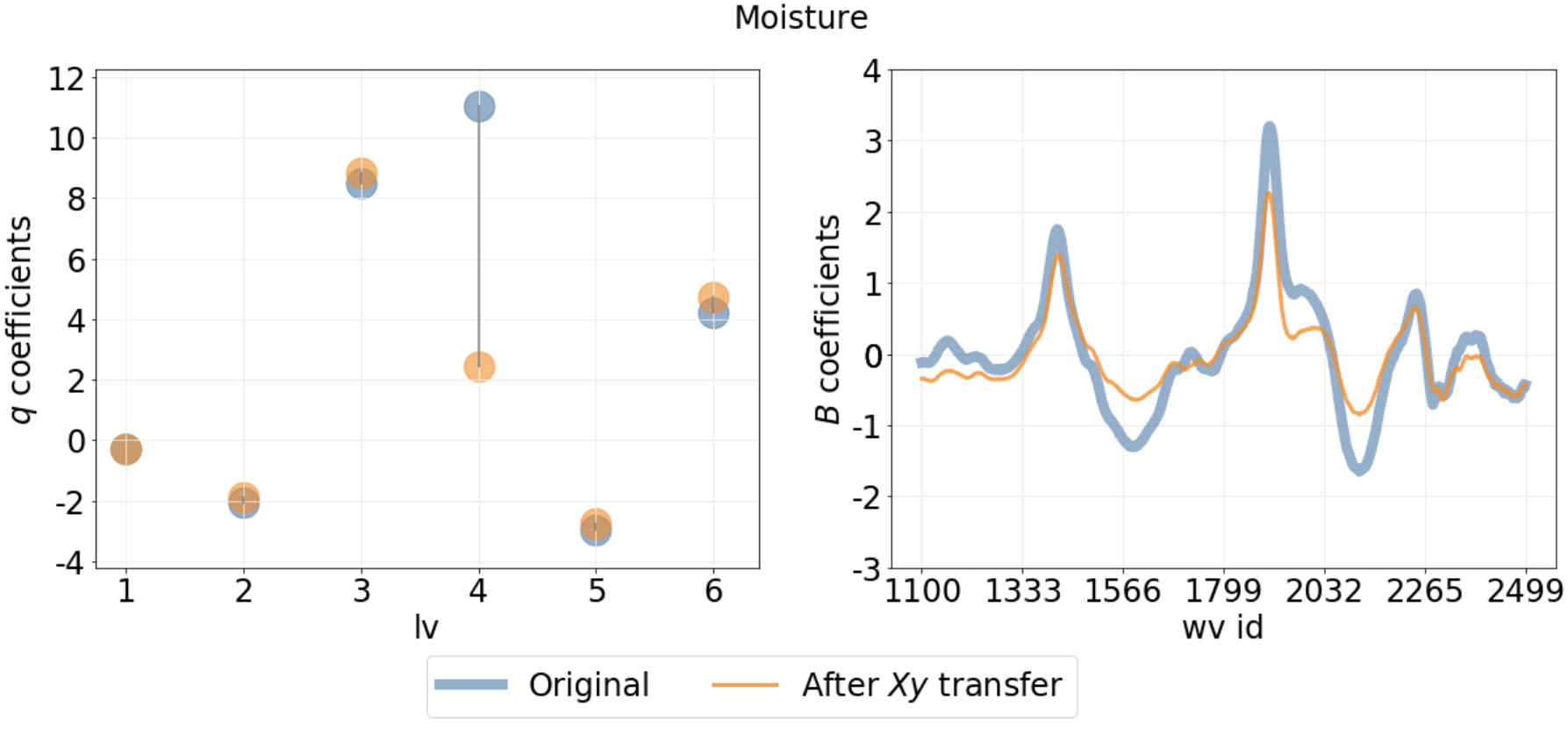
$$|var(\mathbf{t}_s) - var(\mathbf{t}_t)| = 0$$

Instrument transfer level



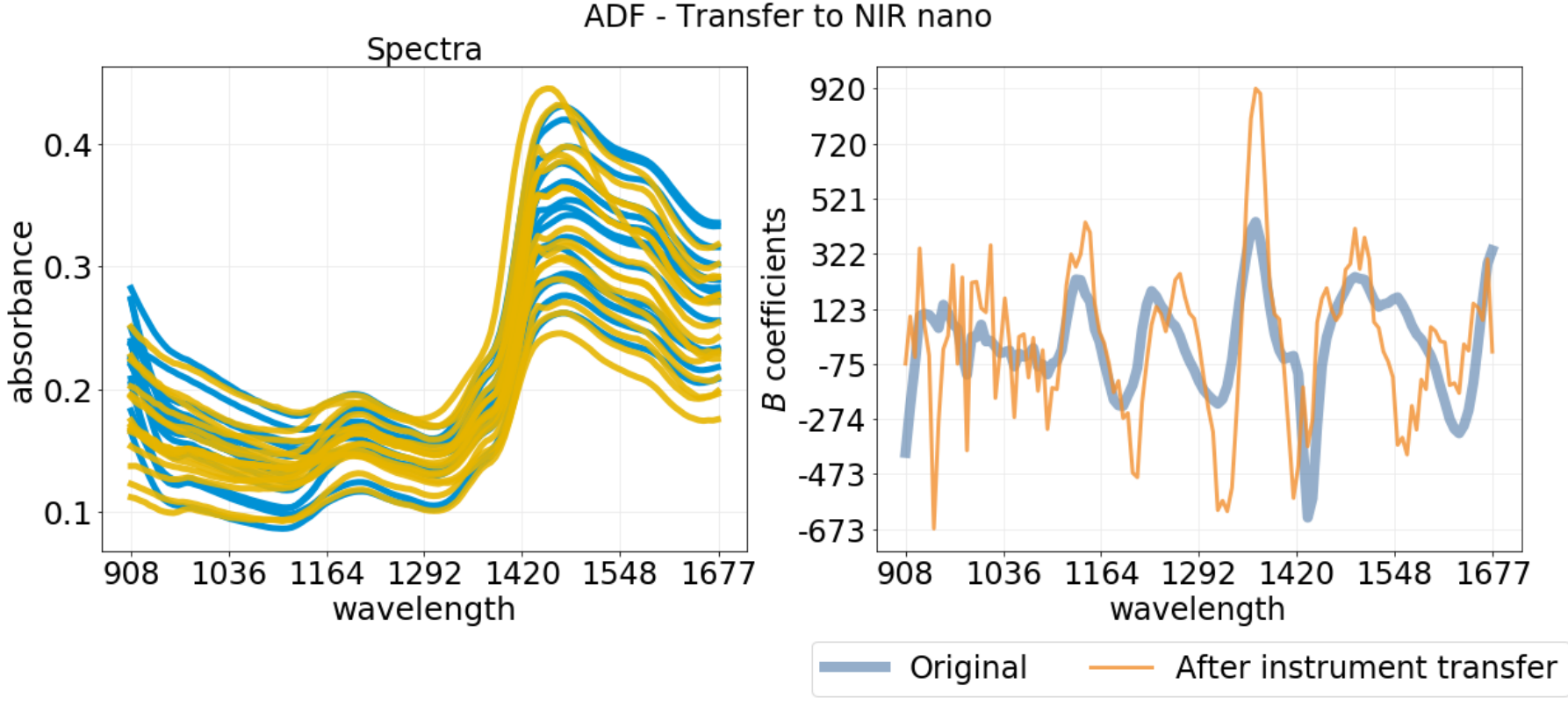
Corn Moisture Content

Original model		Transferred model		
RMSEP	R_p^2	Technique	RMSEP	R_p^2
0.0354	0.9915	Joint Y PLS	0.1701	0.8029



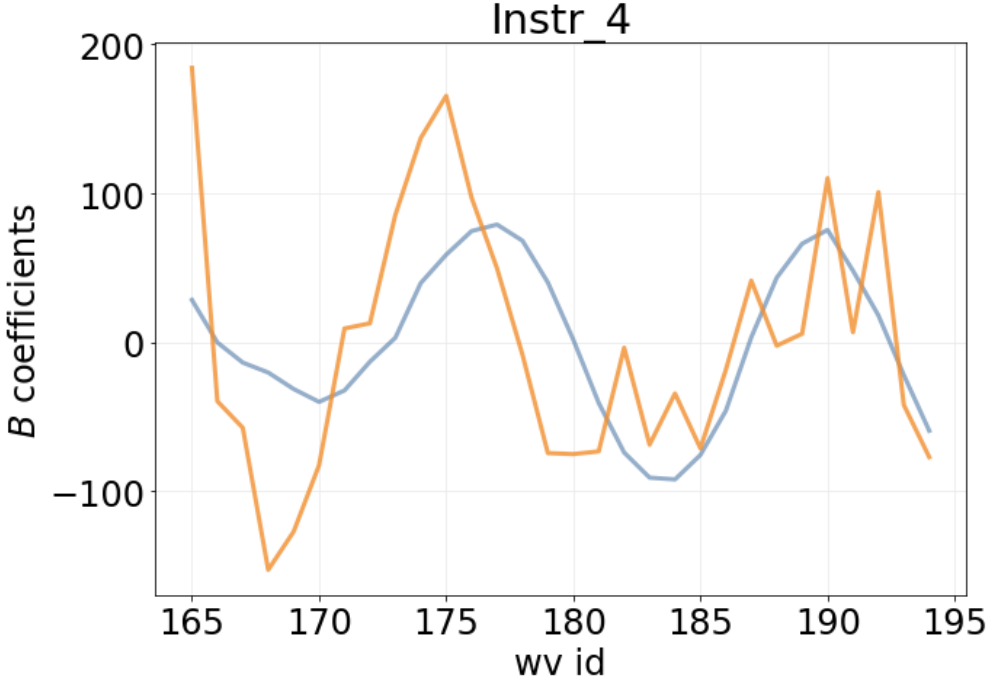
Sugarcane Acid Detergent Fiber Fraction (ADF)

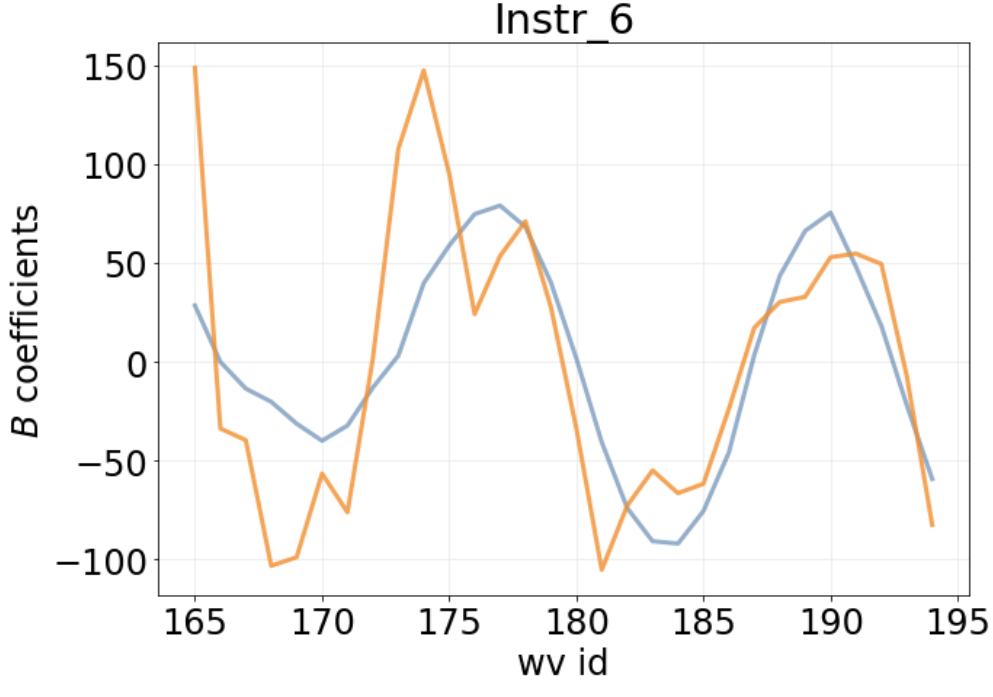
Micro NIR 1700		Micro NIR 1700 - NIR nano		
RMSEP	R_p^2	**Technique**	**RMSEP**	R_p^2
3.6304	0.8613	Orthogonalization	4.5343	0.7837



Brix Pears (e-Chimiométrie 2021)

SNV + Orthogonalization		SNV + DIPLS (unsupervised)											
Winner		**Instr 2**		**Instr 3**		**Instr 4**		**Instr 5**		**Instr 6**		**Instr 7**	
RMSEP	R_p^2	**RMSEP**	R_p^2	**RMSEP**	R_p^2	**RMSEP**	R_p^2	**RMSEP**	R_p^2	**RMSEP**	R_p^2	**RMSEP**	R_p^2
0.7960	0.8520	0.6554	0.8773	0.5480	0.9042	0.5730	0.9026	0.7244	0.8473	0.5457	0.9205	0.5388	0.9113





RECOMMENDATIONS FOR A SUCCESSFUL TRANSFER

Control transfer or degradation of the model separating bias, slope and variance problems

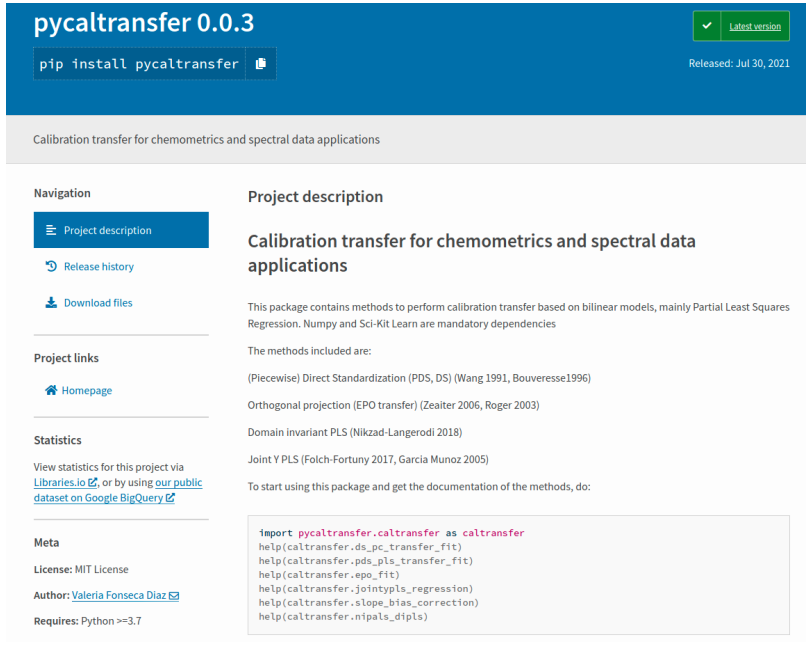
When bias and/or slope are the issue, SBC or Joint Y PLS are helpful methods

Orthogonalization and DIPLS are particularly advantageous when variance is an issue

Instrument standardization is only successful when the relationship between instruments is linear and standard samples are available

SOFTWARE AVAILABILITY

pycaltransfer in Python



pycaltransfer 0.0.3

Latest version

pip install pycaltransfer

Released: Jul 30, 2021

Calibration transfer for chemometrics and spectral data applications

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Statistics

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Meta

License: MIT License

Author: Valeria Fonseca Diaz

Requires: Python >=3.7

Project description

Calibration transfer for chemometrics and spectral data applications

This package contains methods to perform calibration transfer based on bilinear models, mainly Partial Least Squares Regression. Numpy and Sci-Kit Learn are mandatory dependencies

The methods included are:

(Piecewise) Direct Standardization (PDS, DS) (Wang 1991, Bouveresse1996)

Orthogonal projection (EPO transfer) (Zeaiter 2006, Roger 2003)

Domain invariant PLS (Nikzad-Langerodi 2018)

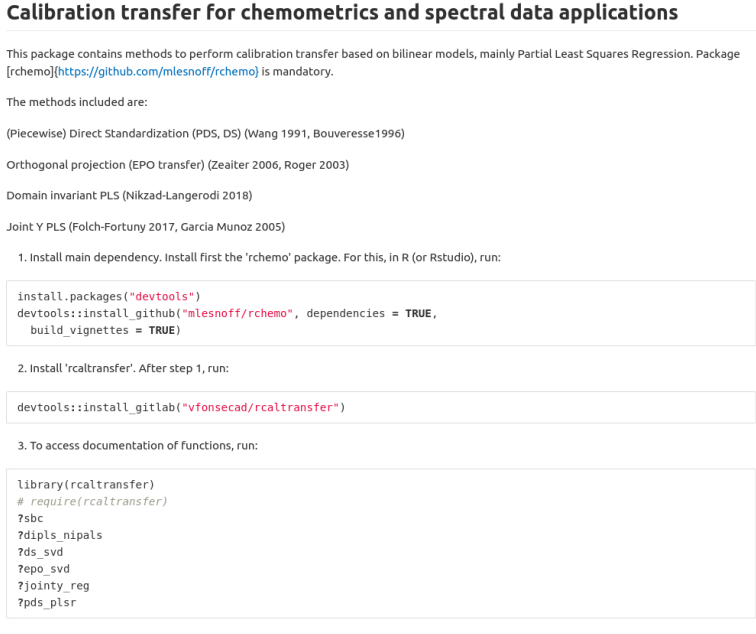
Joint Y PLS (Folch-Fortuny 2017, Garcia Munoz 2005)

To start using this package and get the documentation of the methods, do:

```
import pycaltransfer.caltransfer as caltransfer
help(caltransfer.ds_pc_transfer_fit)
help(caltransfer.pds_pls_transfer_fit)
help(caltransfer.epo_fit)
help(caltransfer.jointypls_regression)
help(caltransfer.slope_bias_correction)
help(caltransfer.nipals_dipls)
```

https://gitlab.com/chemsoftware/python/pycaltransfer

rcaltransfer in R



Calibration transfer for chemometrics and spectral data applications

This package contains methods to perform calibration transfer based on bilinear models, mainly Partial Least Squares Regression. Package [rchemo]{https://github.com/mlesnoff/rchemo} is mandatory.

The methods included are:

(Piecewise) Direct Standardization (PDS, DS) (Wang 1991, Bouveresse1996)

Orthogonal projection (EPO transfer) (Zeaiter 2006, Roger 2003)

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Joint Y PLS (Folch-Fortuny 2017, Garcia Munoz 2005)

1. Install main dependency. Install first the 'rchemo' package. For this, in R (or Rstudio), run:

```
install.packages("devtools")
devtools::install_github("mlesnoff/rchemo", dependencies = TRUE,
  build_vignettes = TRUE)
```

2. Install 'rcaltransfer'. After step 1, run:

```
devtools::install_gitlab("vfonsecad/rcaltransfer")
```

3. To access documentation of functions, run:

```
library(rcaltransfer)
# require(rcaltransfer)
?sbc
?dipls_nipals
?ds_svd
?epo_svd
?jointy_reg
?pds_plsr
```

https://gitlab.com/chemsoftware/rproject/r

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