

A REVIEW OF CALIBRATION TRANSFER AND MAINTENANCE IN AN UNSUPERVISED WAY

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WHAT IS CALIBRATION TRANSFER?

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

Calibration transfer may refer to retaining and reusing a source calibration model and/or the source calibration data to achieve an adaptation obtaining a target calibration model.

Methodology	Types of samples		
Category	Standards	Target spectra and reference values	Only target spectral measurements
Linear standardization	DS, PDS		Spectral mean correction
Prediction correction		SBC	
Concatenation	Joint PCA	Joint PLS	
Orthogonalization	TOP	DOP	uDOP
Variable selection	CAWS		di-CovSel
Domain invariant		Supervised di-PLS	Unsupervised di-PLS

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1. SPECTRAL MEAN CORRECTION

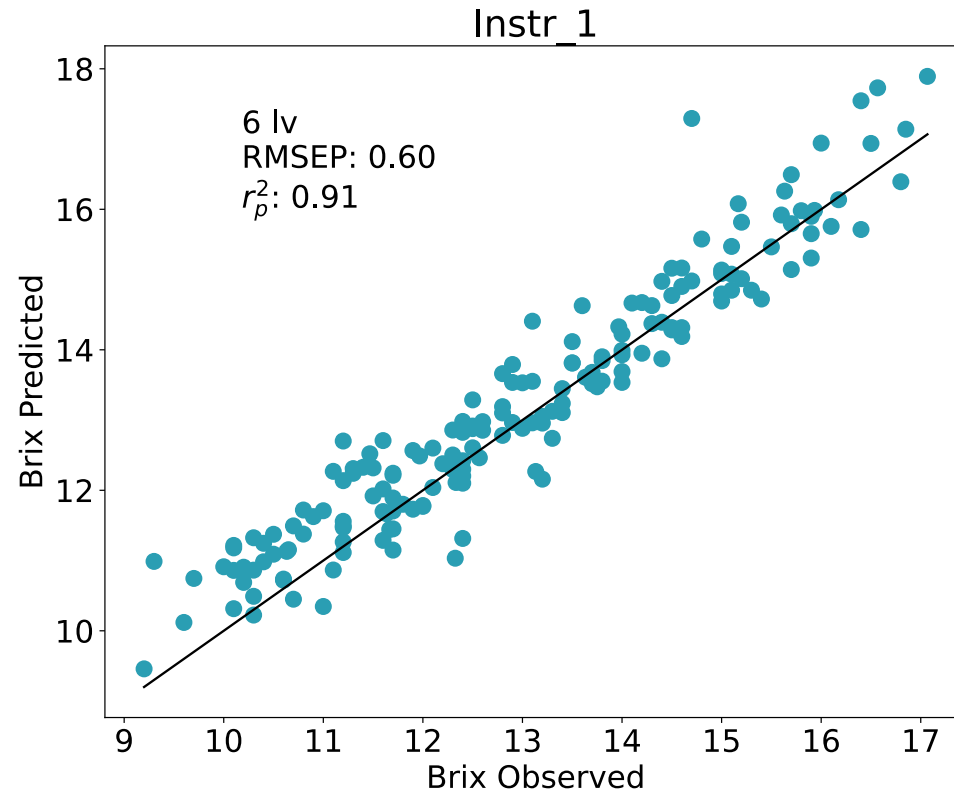
$$y_s = X_s B_s + \beta_s$$

$$\beta_s = \bar{y} - B'_s \bar{X}_s$$

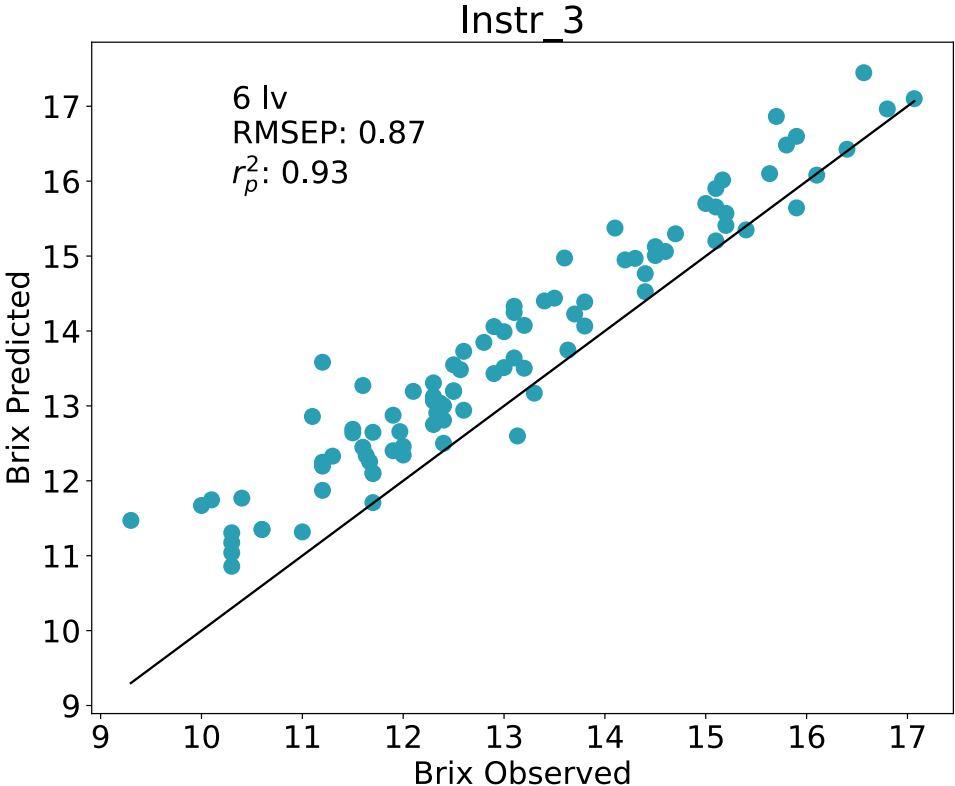
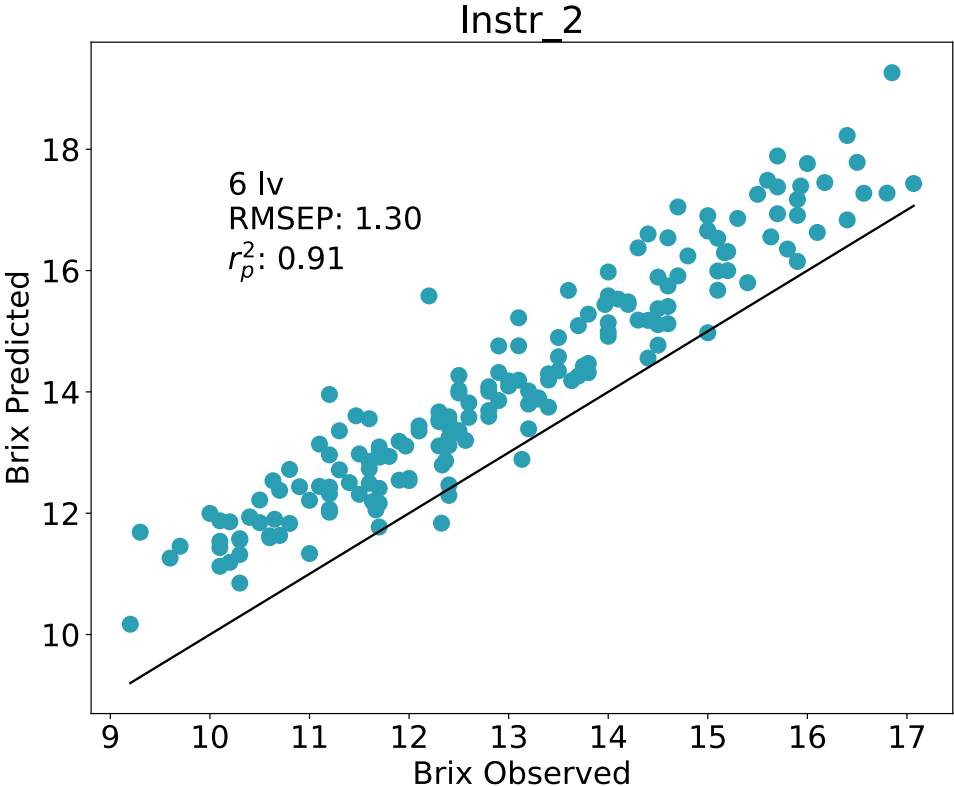
$$\beta_t = \bar{y} - B'_s \bar{X}_t$$

$$y_t = X_t B_s + \beta_t$$

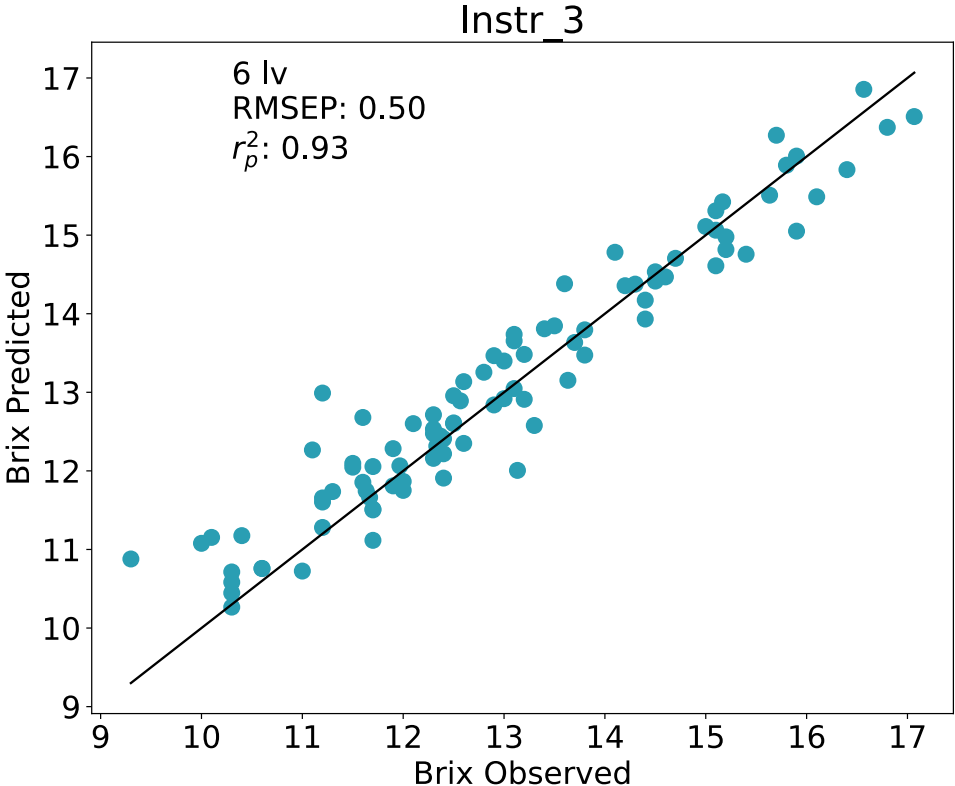
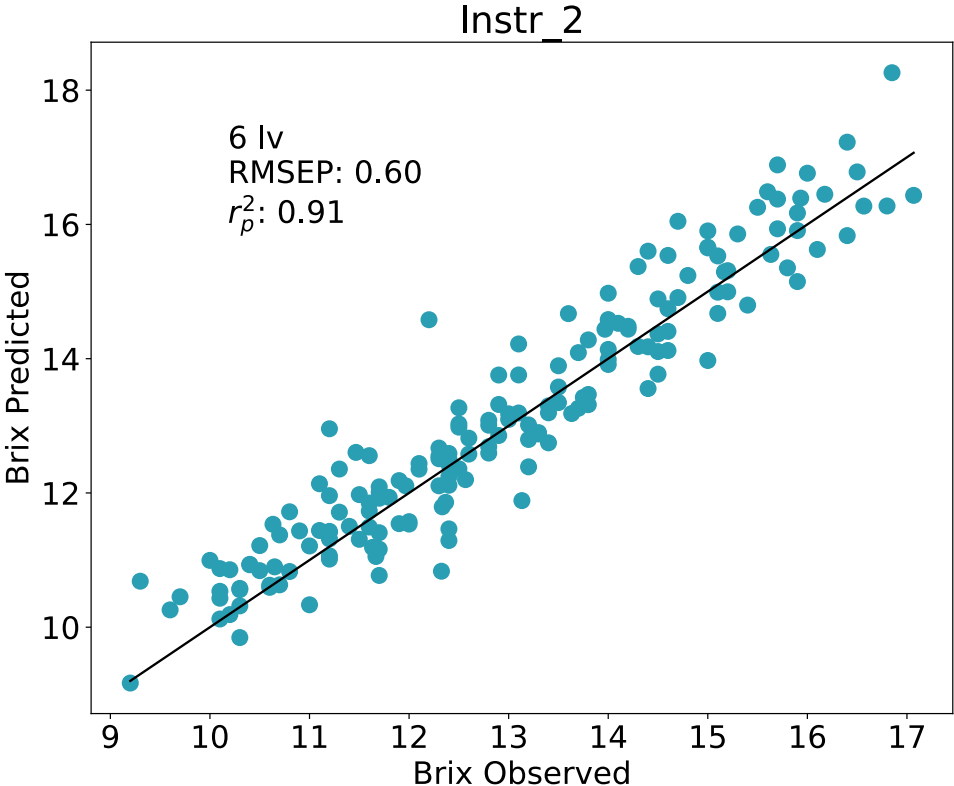
BRIX PREDICTION IN PEARS FOR MULTIPLE INSTRUMENTS



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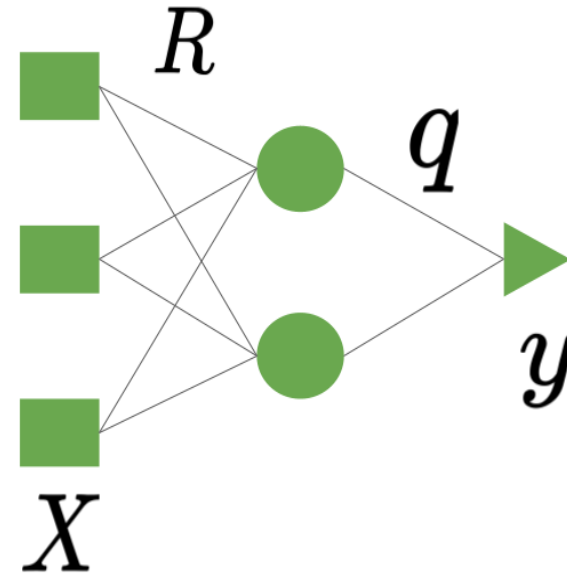
2. CALIBRATION USING DOMAIN INVARIANT PLS (Nikzad-Langerodi, R. et al. 2018)

Optimize

$$\min_w ||X - yw^T||$$

subject to:

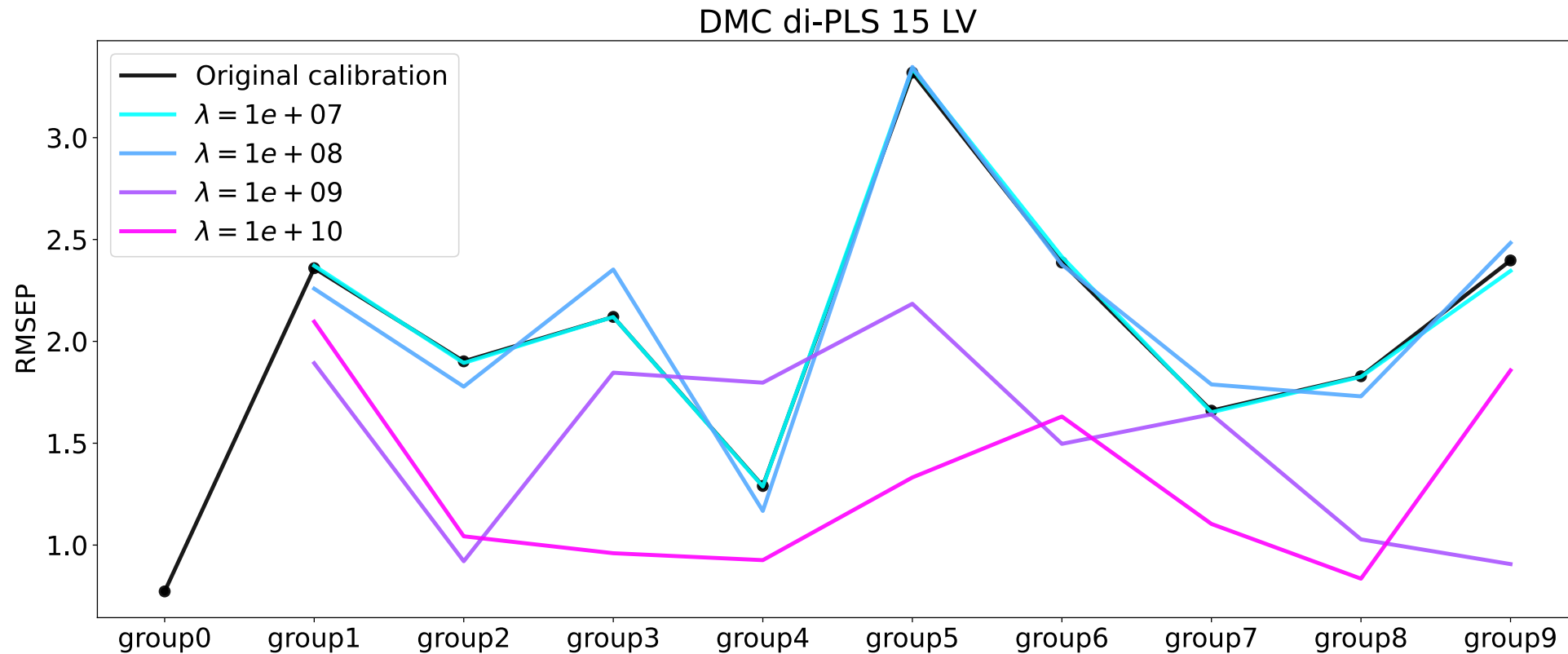
$$|var(\mathbf{t}_s) - var(\mathbf{t}_t)| = 0$$



DRY MATTER CONTENT PREDICTION IN MANGO SAMPLES

Domain	Type	Cultivar	Season	<i>n</i>
Source	Hard Green	Caly	1	1277
Target 1	Hard Green	KP	1	1059
Target 2	Hard Green	HG	1	293
Target 3	Hard Green	KP	2	340
Target 4	Hard Green	HG	2	88
Target 5	Hard Green	R2E2	2	276
Target 6	Hard Green	KP	3	216
Target 7	Hard Green	HG	3	80
Target 8	Hard Green	R2E2	3	156
Target 9	Ripen	KP	3	78

DRY MATTER CONTENT PREDICTION IN MANGO SAMPLES FROM SEVERAL DOMAINS



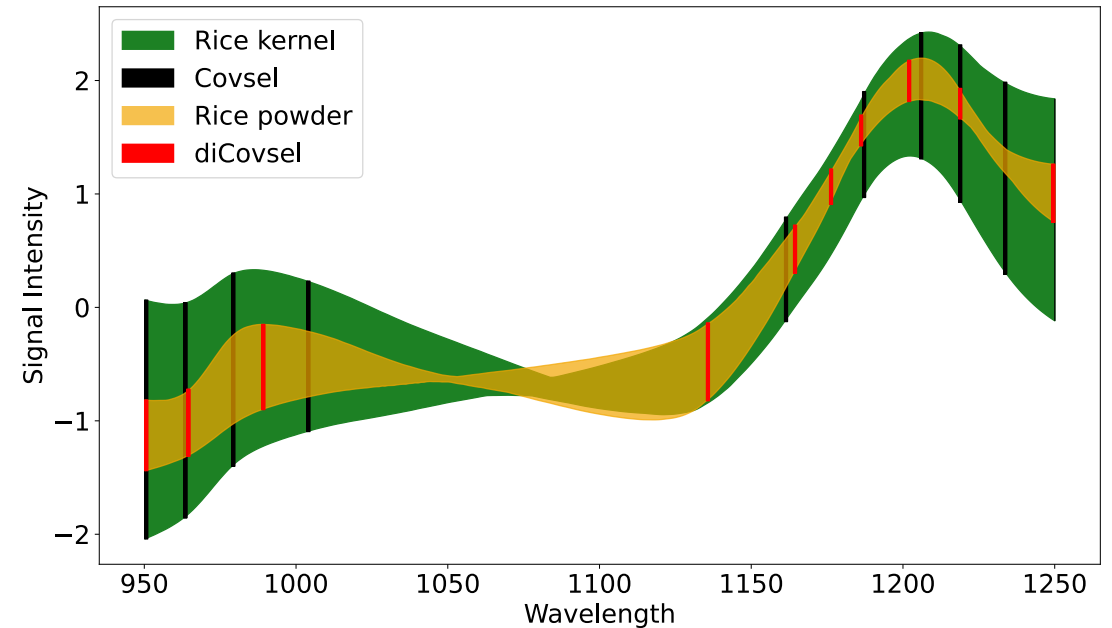
3. VARIABLE SELECTION USING DOMAIN INVARIABILITY (DI-COVSEL) (Diaz, V.F., et al. 2022)

Optimize

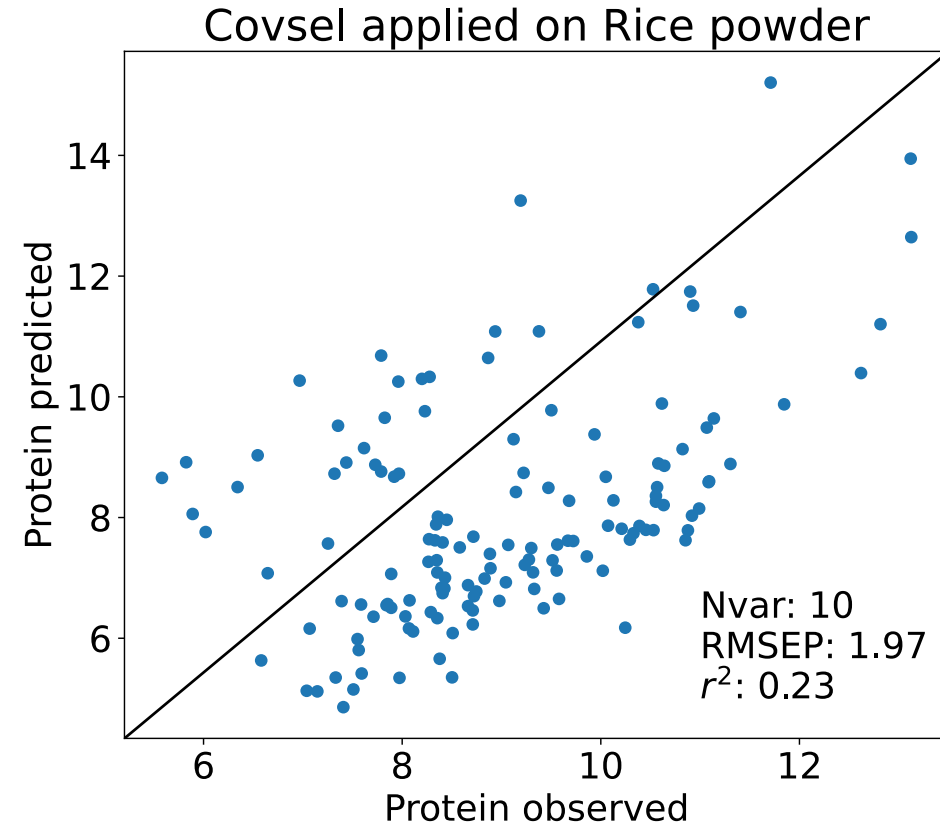
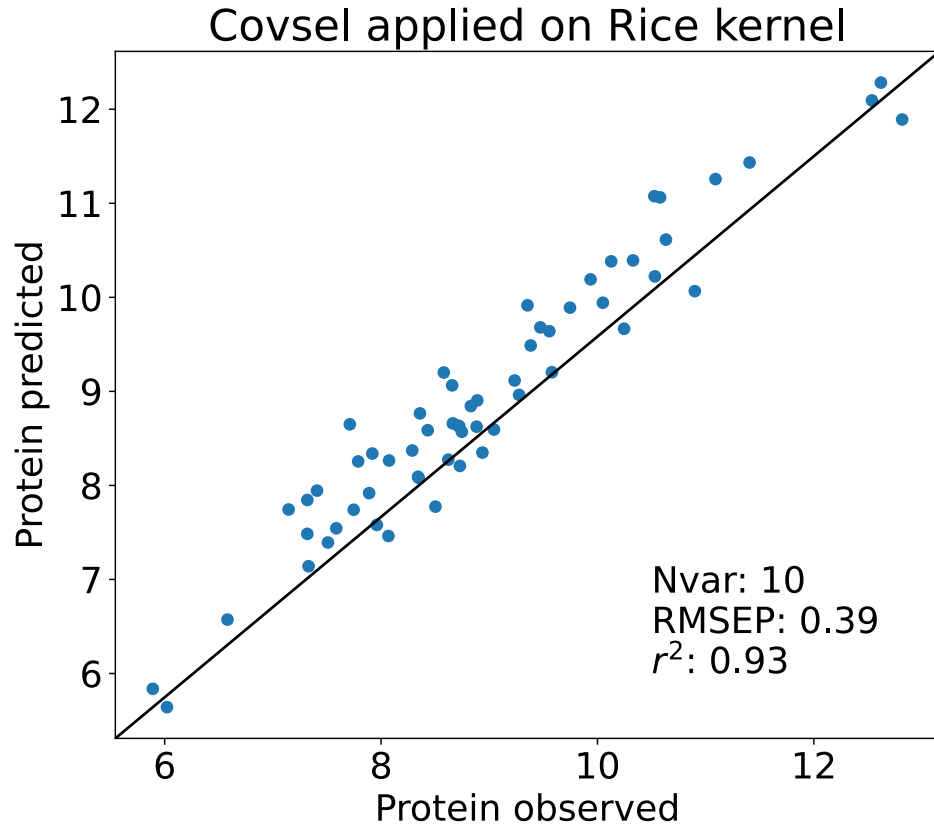
$$\max_j \text{cov}^2(a_j x_j, y)$$

where:

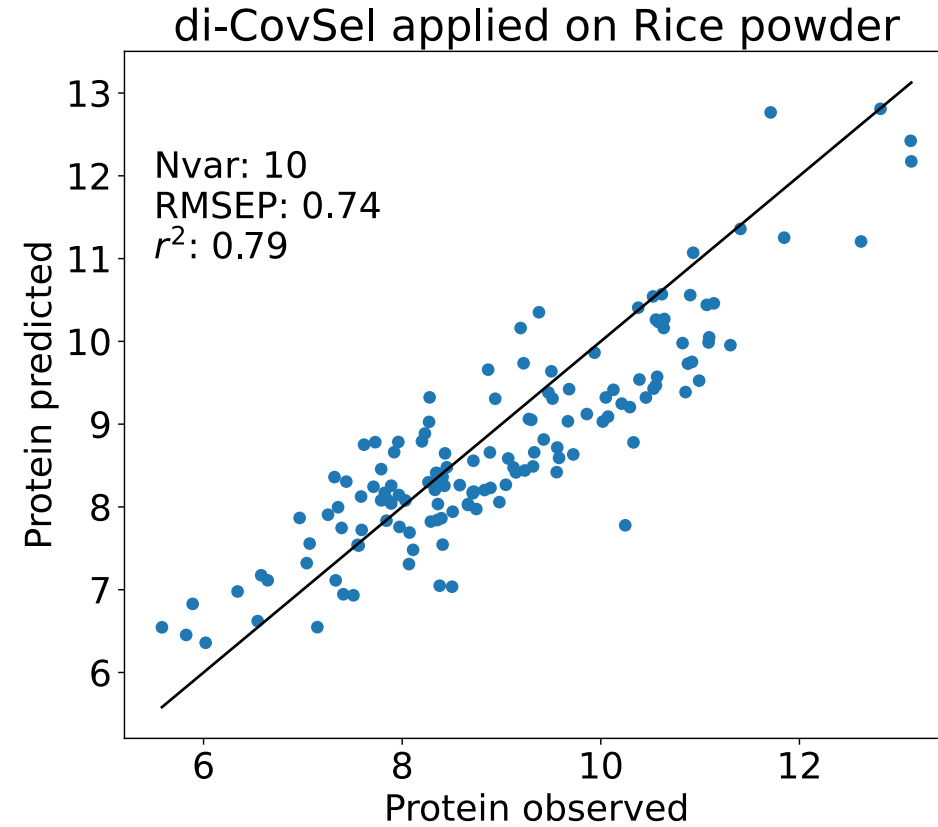
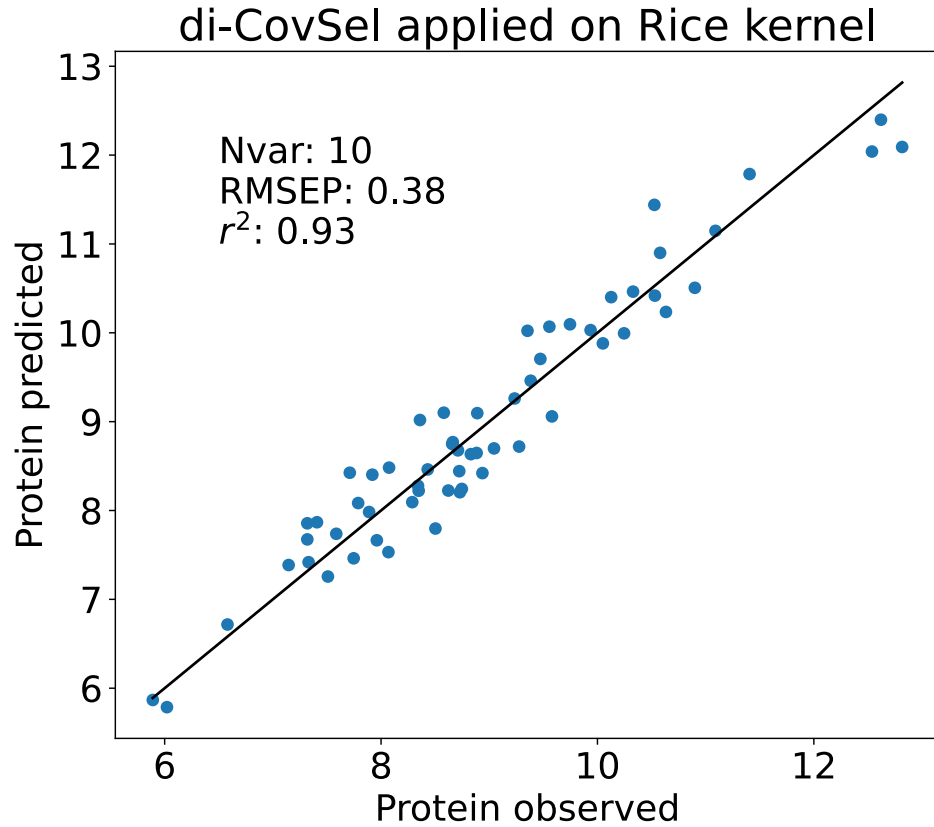
$$A = f(\text{cov}(X_s) - \text{cov}(X_t))$$



PROTEIN CONTENT PREDICTION IN TWO RICE FORMS



PROTEIN CONTENT PREDICTION IN TWO RICE FORMS



RECOMMENDATIONS

Think of calibration transfer as an adaptation of the model rather than an equalization of domains (instruments)

Study the type of degradation experienced by the source model in the target domain

Consider the different methodology categories rather than specific methods to decide on the types of samples needed

SOFTWARE AVAILABILITY

pycaltransfer

pycaltransfer 0.1.6 Latest version
`pip install pycaltransfer` Released: Mar 24, 2022

Calibration transfer for chemometrics and spectral data applications

Navigation

- Project description
- Release history
- Download files

Project links

- Homepage

Statistics

View statistics for this project via [Libraries.io](#), or by using [our public dataset on Google BigQuery](#)

Meta

License: MIT License

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, 2020)
- Joint Y PLS (Folch-Fortuny 2017, Garcia Munoz 2005)
- Spectral Space Transformation (SST) (W. Du, 2011)
- Transfer by orthogonal projection (TOP) (A. Andrew and T. Fearn, 2004)
- Dynamic orthogonal projection (DOP) (Zeater, et al 2006)
- Transfer component analysis (TCA) (Pan, et al 2011)

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

chemdemos

ChemSoftware > InPython

InPython Group ID: 13619781

Subgroups and projects | Shared projects | Archived projects

- C chemdemos** This is a list of demos for chemometrics methodology
- D dicovsel** This is the repository for Domain Invariant Covariate Selection
- P pycaltransfer** Calibration transfer recopilation of state of the art

<https://gitlab.com/chemsoftware/python/chemdemos>

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