

Exploring the relationship between sensory and instrumental data with component-based methods



**KoSFiST International Symposium
and Annual Meeting 2025**

Pioneering Future Connection in FoodTech
Gwangju, Korea · 2-4 July 2025

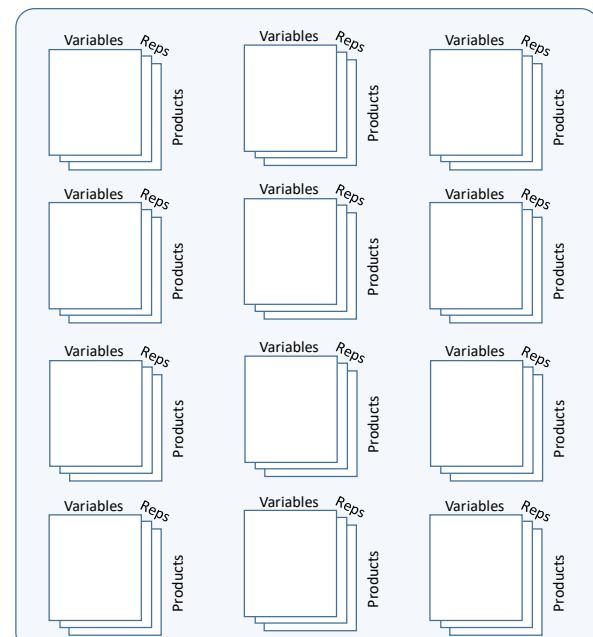
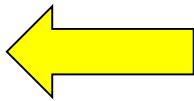
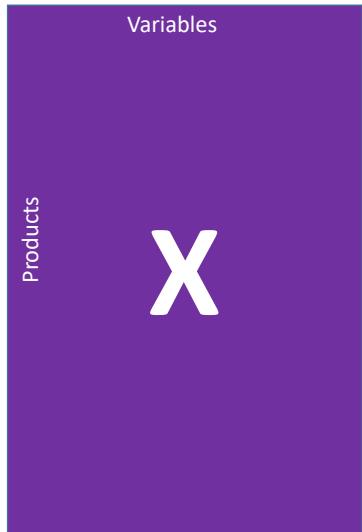
John Castura

Dr. Philos., M.Sc.
Research Fellow

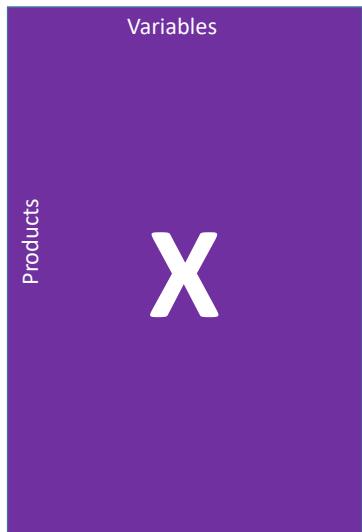




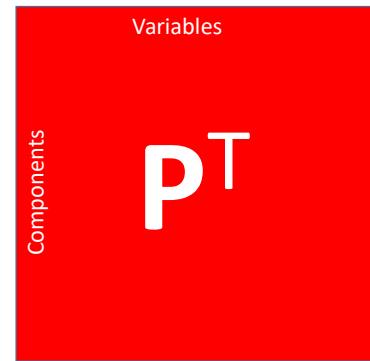
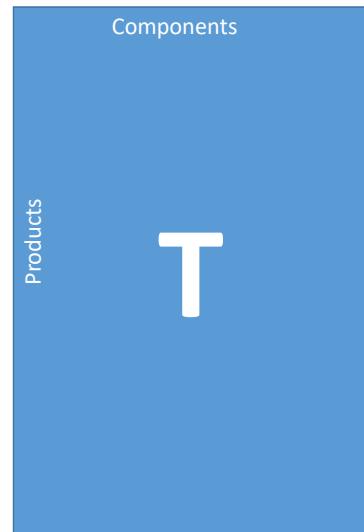
Aggregate into data matrix



Principal component analysis



=



Dimension reduction to A components

$$X = T_A P_A^T + \text{Residual}$$

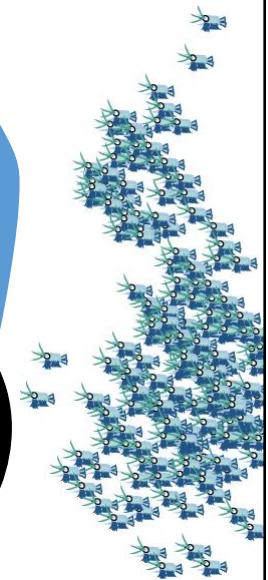
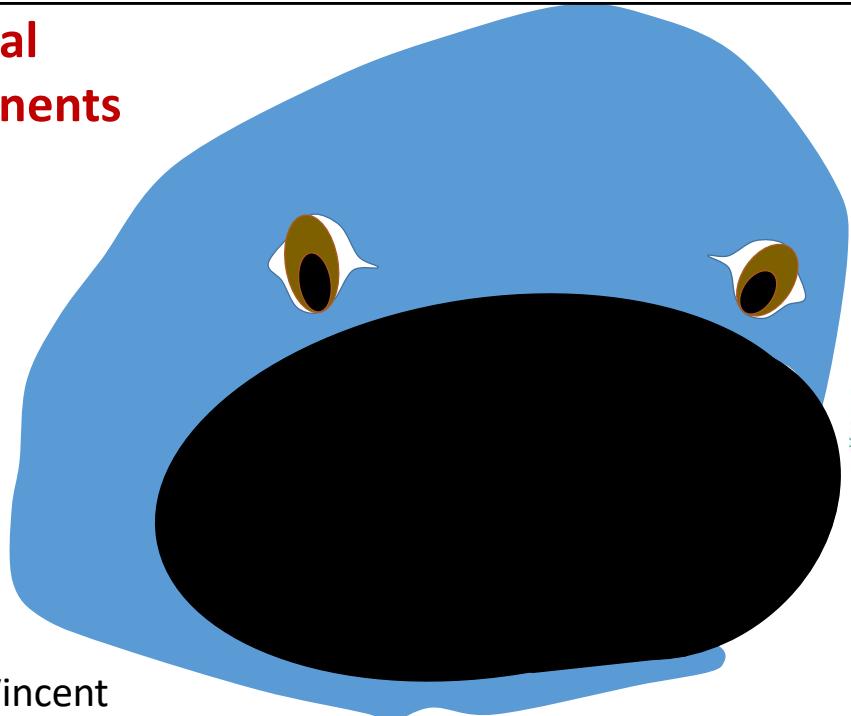


Principal components

Baleen whale



*merci Vincent



Dimension reduction

X

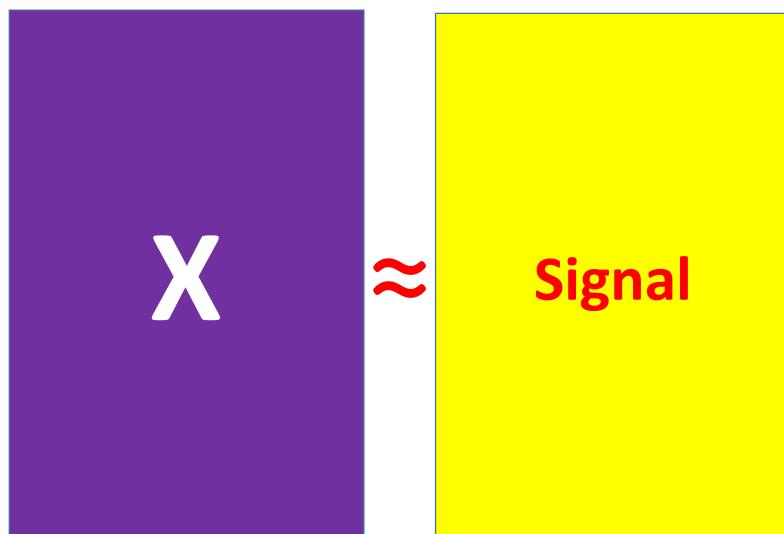
=

Signal

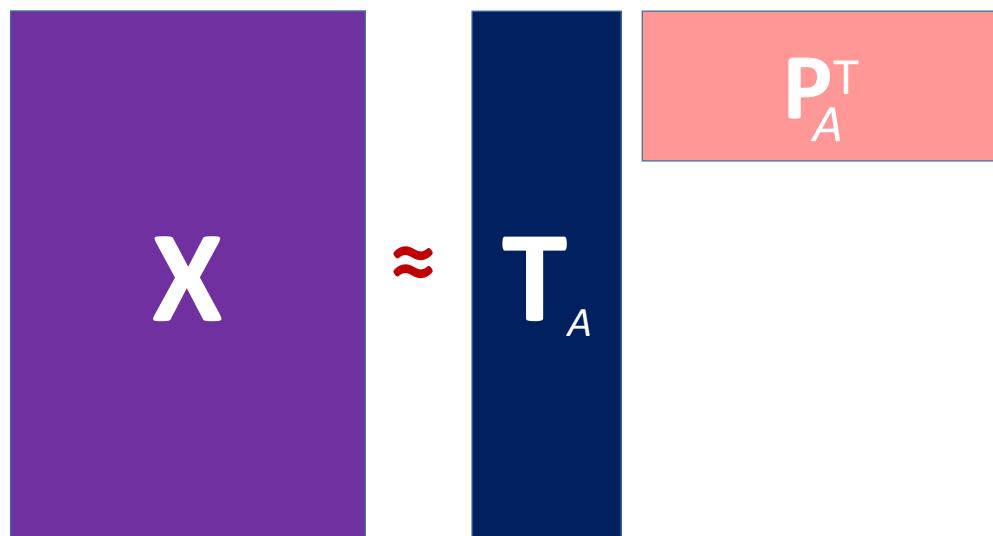
+

Noise

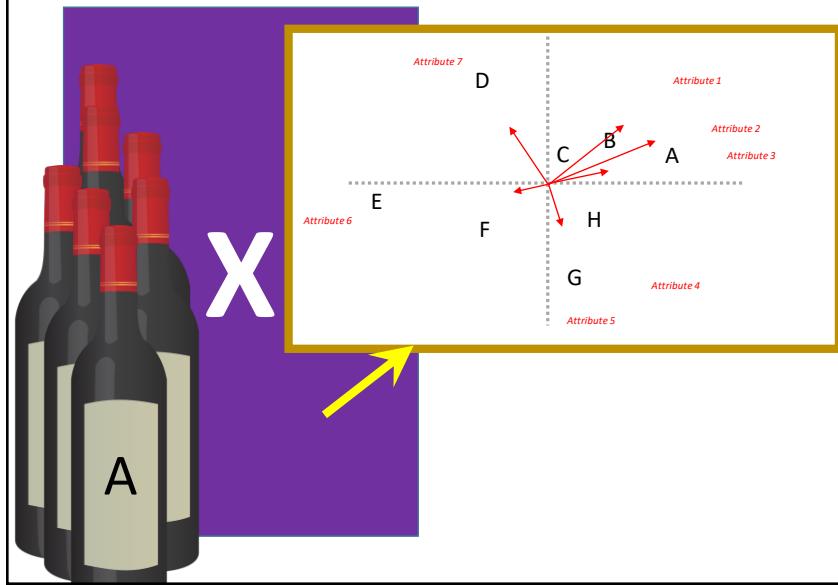
Dimension reduction



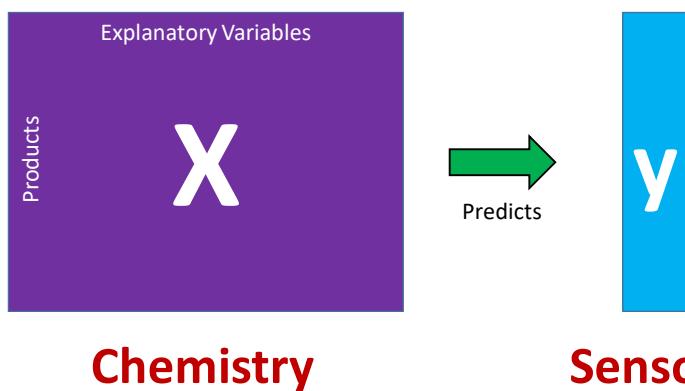
Dimension reduction to A components



Visualizing PCA results



Investigating data relationships



Why component-based methods?

- Summarize and visualize complicated data
- Often relatively few underlying sources of variation
- Useful approximation of data
- Separation of signal/noise
- Outlier detection
- Confirm hypotheses
- Generate hypotheses

Næs, Varela, Castura, Bro & Tomic (2023). Why use component-based methods in sensory science? *Food Quality and Preference*, 112, 105028.
<https://doi.org/10.1016/j.foodqual.2023.105028>

Data for French Pinot Noir Wines

Volatile organic compounds (VOCs)

Headspace measurements of VOCs obtained from
headspace—solid phase micro-extraction—gas chromatography—mass spectrometry (HS-SPME-GC-MS)

X	1-hexanol	acetaldehyde	ethyl acetate	isoamyl acetate
	1-octanol	acetic acid	ethyl butyrate	isoamyl propionate
	1-phenoxy-2-propanol	alpha-ionone	ethyl caproate	isovaleric acid
	2,3-butanedione	beta-ionone	ethyl isobutyrate	methional
	2-ethylhexan-1-ol	butyl acetate	ethyl isovalerate	methionol
	2-isobutyl-3-methoxypyrazine	butyric acid	ethyl lactate	pentyl propionate
	2-methyl-1-butanol	damascenone	ethyl octanoate	phenol
	2-methylbutyl acetate	dimethyl sulfide	ethyl propionate	phenylacetaldehyde
	2-phenylethanol	ethyl 2-methylbutyrate	furaneol	phenylacetic acid
	3-methyl-1-butanol	ethyl 3-hydroxybutyrate	hexyl acetate	propionic acid
	4-ethyl-2-methoxyphenol	ethyl 6-hydroxyhexanoate	homofuraneol	trans-3-hexen-1-ol
	4-ethylphenol			

Villiére et al. (2019)

Pinot noir wines

T1 2010 Bourgogne PDO

T5 2009 Savigny-lès-Beaune PDO

T2 2009 Bourgogne PDO

T6 2010 Maranges PDO

T3 2009 Bourgogne PDO

C 2009 Côte de Nuits-villages PDO

T4 2009 Bourgogne Hautes Côtes de Beaune PDO

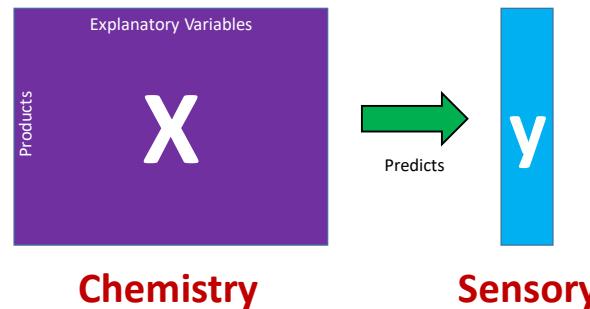
T7 2009 Ladoix PDO

Villiére et al., 2019, <https://doi.org/10.1016/j.dib.2019.103725>

Sensory Variables

Y

Artichoke	Cherry fresh	Hay	Smoky
Bell pepper	Cherry stone	Leather	Strawberry cooked
Blackberry fresh	Clove	Musk	Strawberry fresh
Blackcurrant bud	Cut grass	Pepper	Toasty
Blackcurrant fresh	Elderflower	Plum cooked	Undergrowth
Blueberry fresh	Ethanol	Plum fresh	Vanilla
Brioche	Firestone	Prune	Violet
Butter	Geranium	Raspberry fresh	Woody
Cherry cooked			



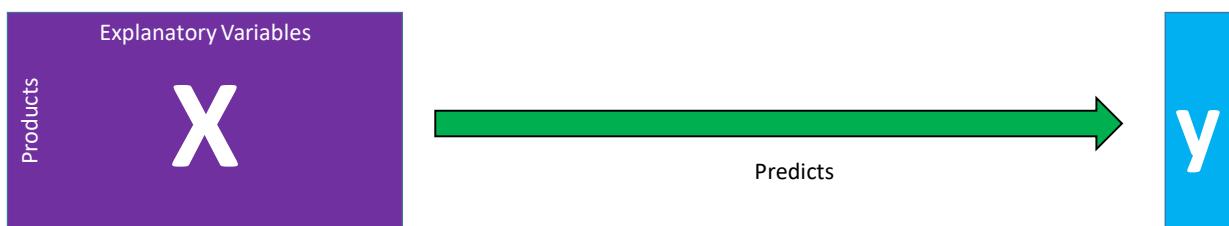
Principal component regression

Unsupervised & Supervised

We want to *predict* the response y from multivariate X .

Response y is regressed on
principal components of X .

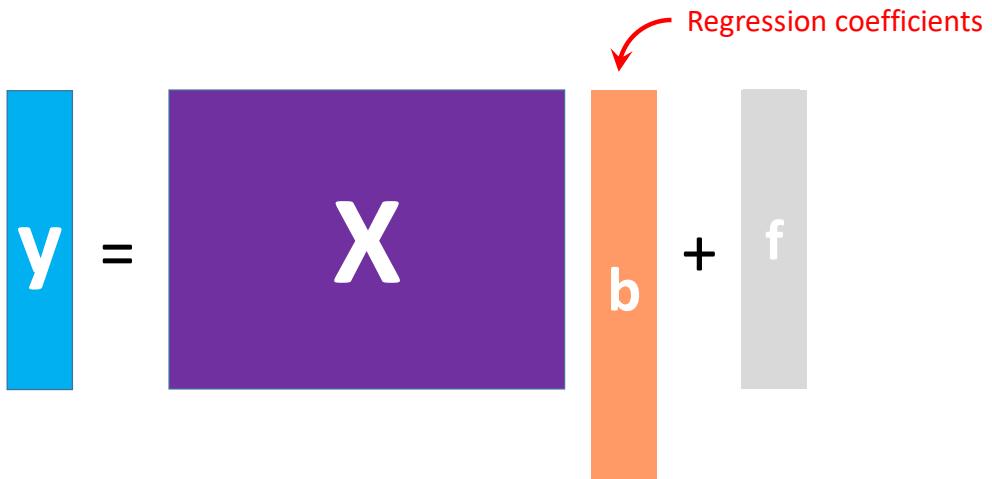
Investigating data relationships with multiple linear regression



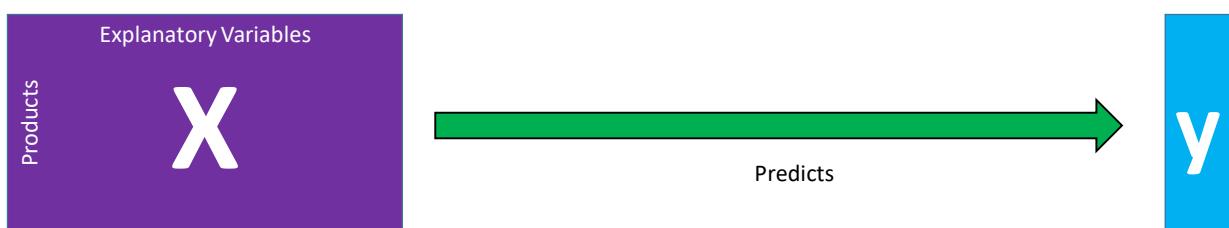
Investigating data relationships with multiple linear regression

$$\mathbf{y} = \mathbf{X} \mathbf{b} + \mathbf{f}$$

Regression coefficients



Investigating data relationships with multiple linear regression

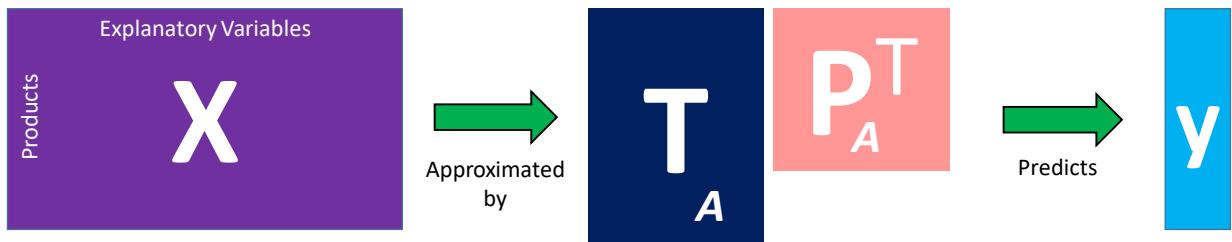


$$\mathbf{y} = \mathbf{X}\mathbf{b} + \mathbf{f}$$
$$\mathbf{b} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Multicollinearity?
More variables than objects?

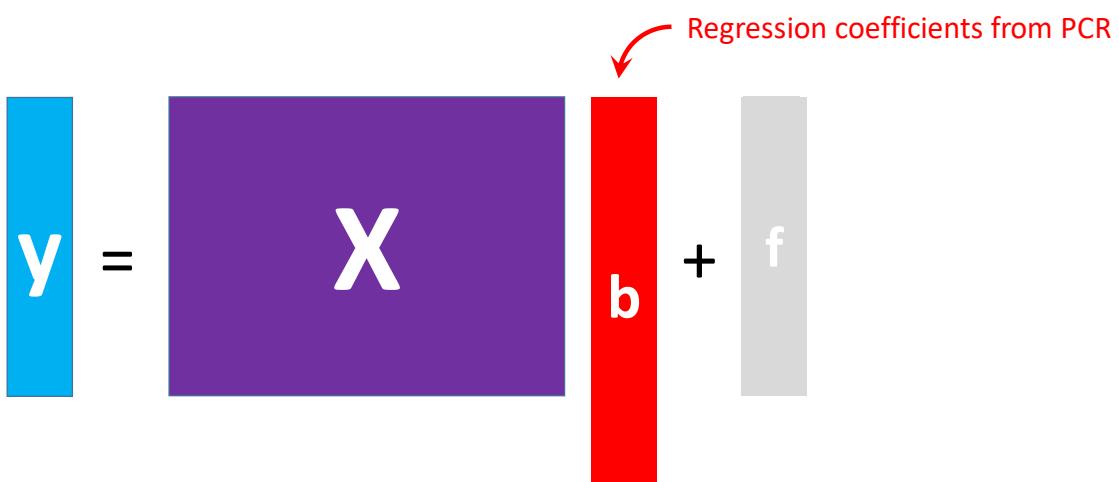
Investigating data relationships

with principal component regression (PCR)

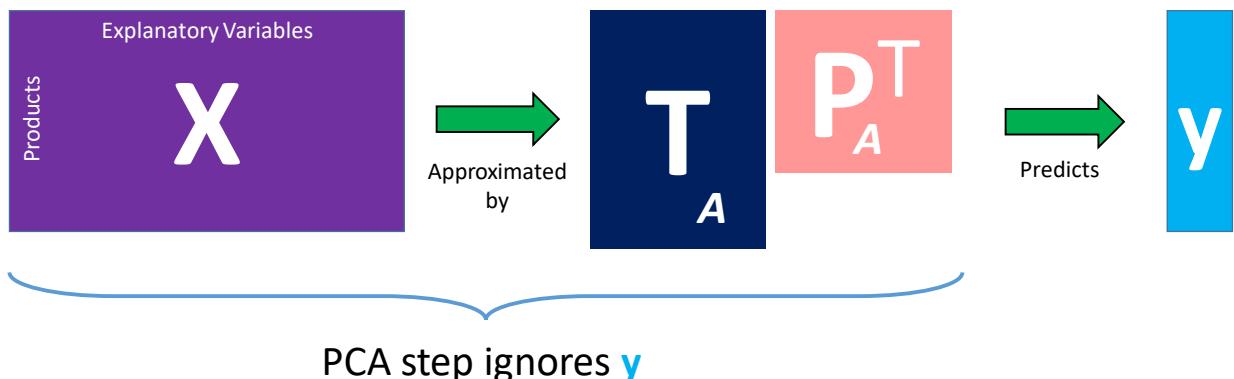


Investigating data relationships

with principal component regression (PCR)



Investigating data relationships with principal component regression (PCR)

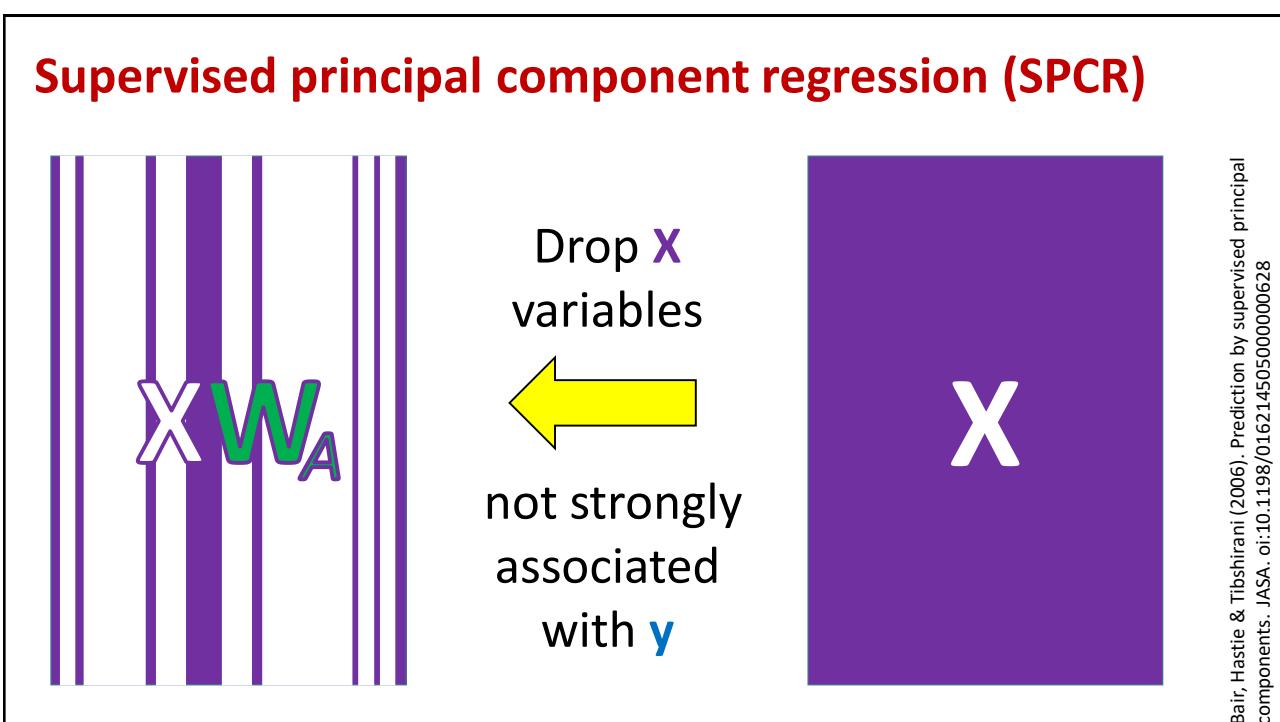
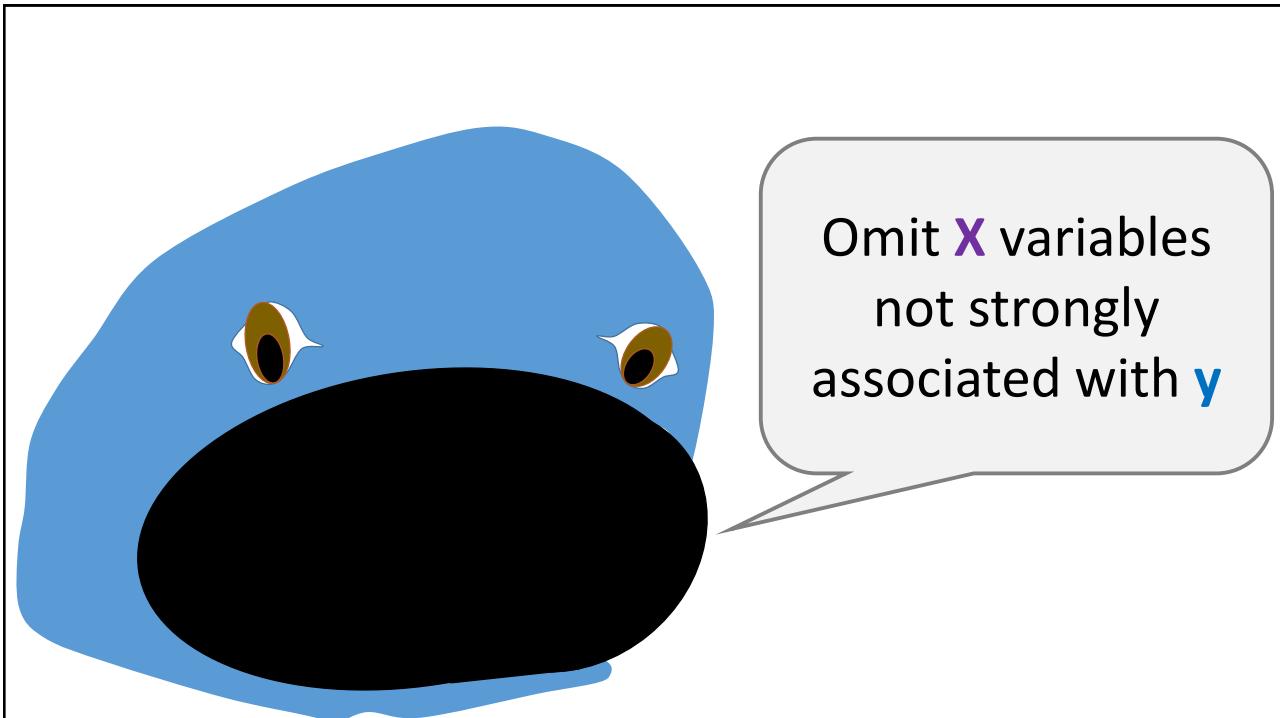


Supervised principal component regression (SPCR)

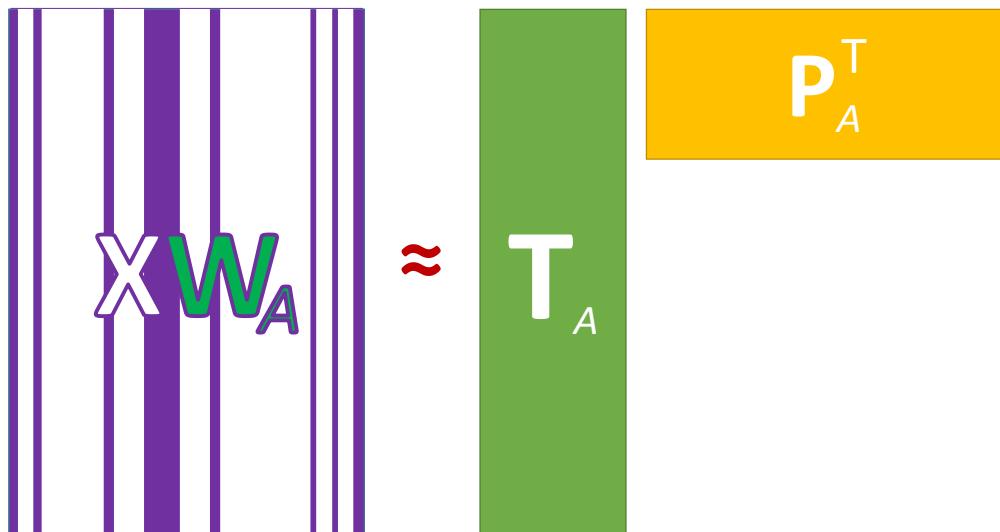
We want to *predict* the response y from the multivariate X .

Response y is regressed on principal components of X .

SUPERVISED

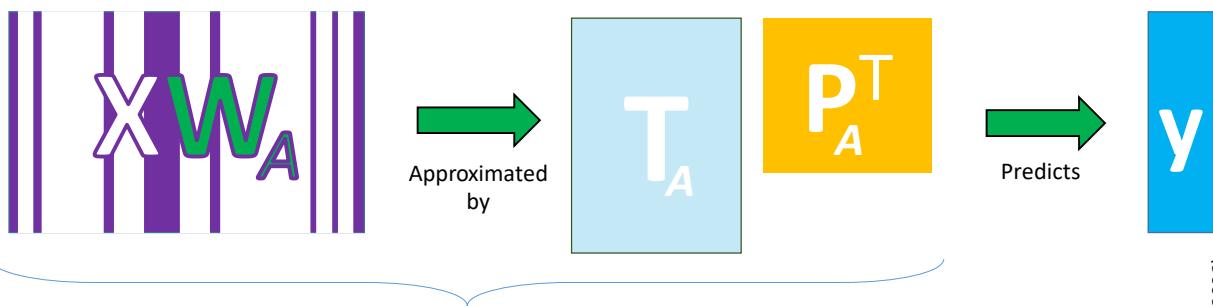


Dimension reduction in SPCR



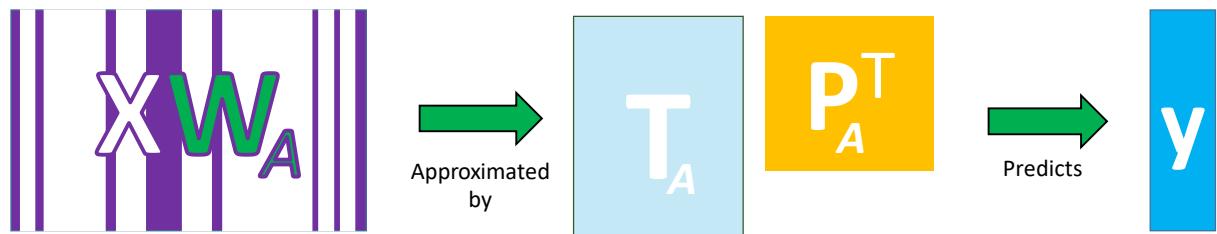
Bair, Hastie & Tibshirani (2006)

Supervised principal component regression (SPCR)



Bair, Hastie & Tibshirani (2006)

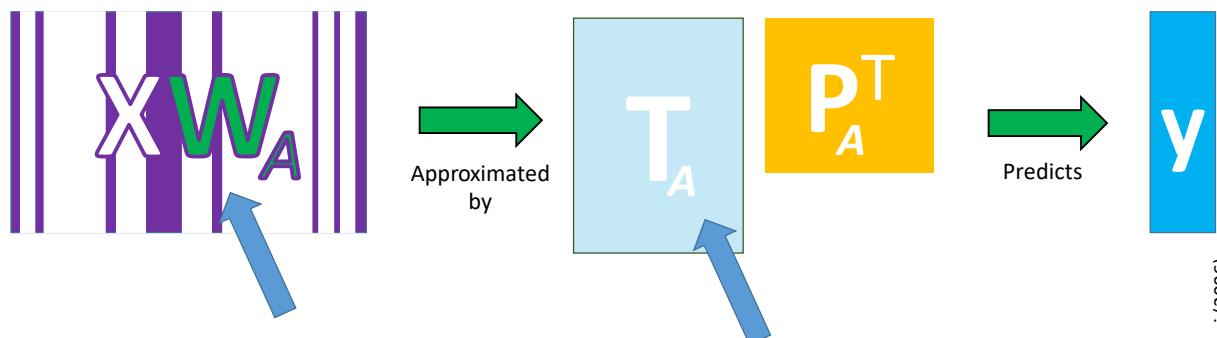
Supervised principal component regression (SPCR)



PCA of filtered X variables yields
Supervised Principal Components

Bair, Hastie & Tibshirani (2006)

Supervised principal component regression (SPCR)



Slope parameter: θ

Weight is 1 for X variables

associated strongly enough with y
and 0 otherwise.

Components parameter: A

Determines number of components.

Bair, Hastie & Tibshirani (2006)

Many candidate values for parameters θ and A

How to choose?

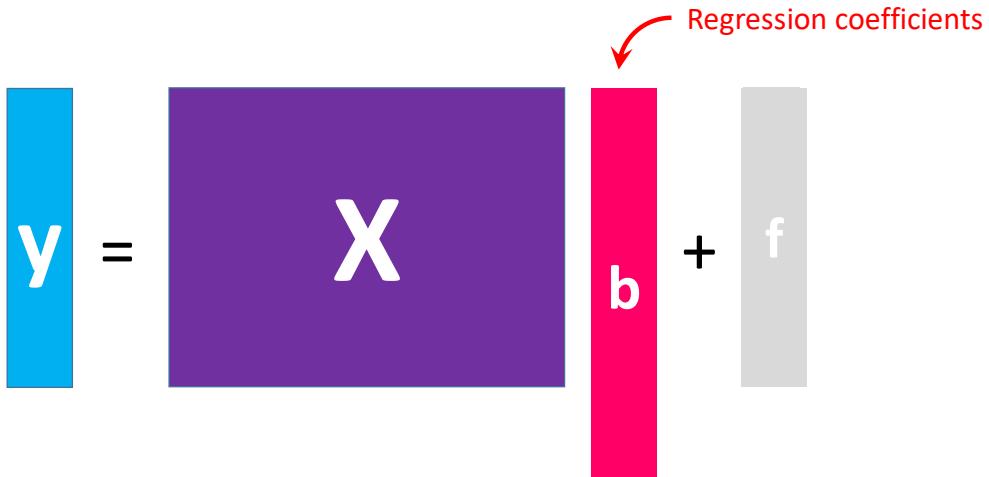
Strategy: Choose model that gives the most accurate predictions for data withheld from model training

Bair et al.: 2-fold cross-validation (2-fold cv)
Us: leave-one-out cross-validation (loocv)

Supervised principal component regression (SPCR)

$$\mathbf{y} = \mathbf{X} \mathbf{b} + \mathbf{f}$$

Regression coefficients



Bair, Hastie & Tibshirani (2006)

Usually, when interpret results, we draw conclusions about...

relationships between variables,

relationships between objects, and

differences between objects.

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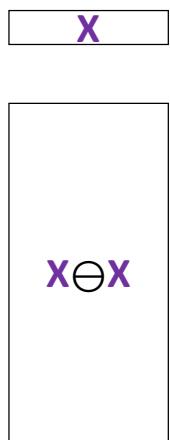
differences between objects.

Investigating paired comparisons after principal component analysis

Castura, J.C., Varela, P, & Næs, T. (2023).
Investigating paired comparisons after principal component analysis. *Food Quality and Preference*, 106, 104814.
<https://doi.org/10.1016/j.foodqual.2023.104814>

Investigating paired comparisons after PCA

“Crossdiff-unfolding”



\mathbf{X} is a column-centered ($J \times M$) matrix

Every row is subtracted from every row

$\mathbf{X} \ominus \mathbf{X}$ is a column-centered ($J^2 \times M$) matrix

Investigating paired comparisons after PCA

“Crossdiff-unfolding”

X

The covariance matrix of X and the covariance matrix of $X \ominus X$ are identical except for a multiplier.

$X \ominus X$

Next, consider PCA of X and PCA of $X \ominus X$.

Investigating paired comparisons after PCA

PCA of X

X

=

blue rectangle

P^T

PCA of $X \ominus X$

$X \ominus X$

=

blue rectangle

P^T

Investigating paired comparisons after PCA

PCA of X

X

=



Key result #1:

Loading matrices obtained from these two PCA solutions are identical.

PCA of $X \ominus X$

$X \ominus X$

=

T

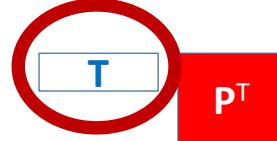


Investigating paired comparisons after PCA

PCA of X

X

=



Key result #2:

If we crossdiff-unfold scores from PCA of X , we get scores from PCA of $X \ominus X$.

PCA of $X \ominus X$

$X \ominus X$

=

$T \ominus T$



Paired comparisons

This demonstrates that objects and all their paired comparisons are optimally investigated
in the same principal components.

Paired comparisons

Therefore, we can just do PCA of \mathbf{X} and know the PCA of $\mathbf{X} \ominus \mathbf{X}$ without actually doing this PCA.

This lays necessary theoretical groundwork to justify a strategy for doing paired comparisons after PCA.

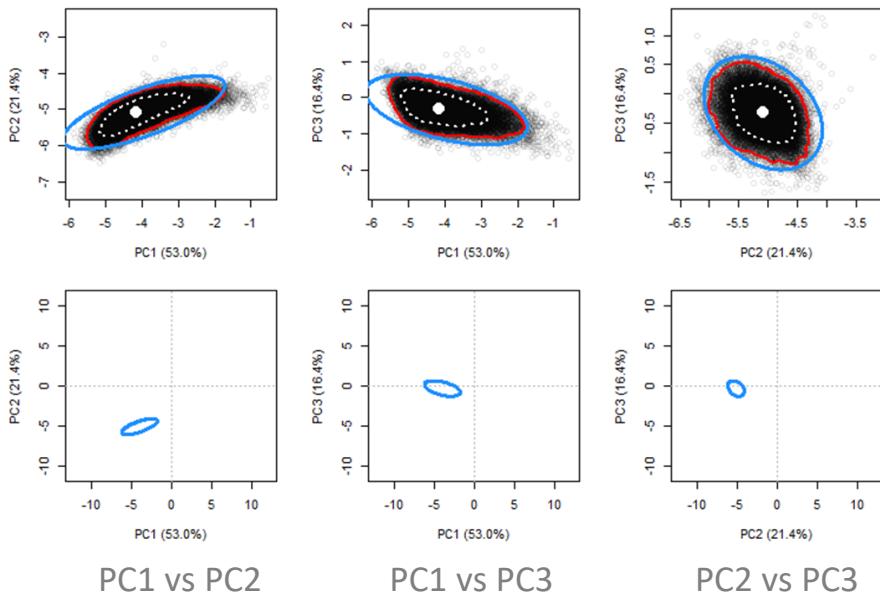
We need to **account for mutual dependencies in the data** when investigating paired comparisons.

Evaluation of complementary numerical and visual approaches for investigating pairwise comparisons after principal component analysis

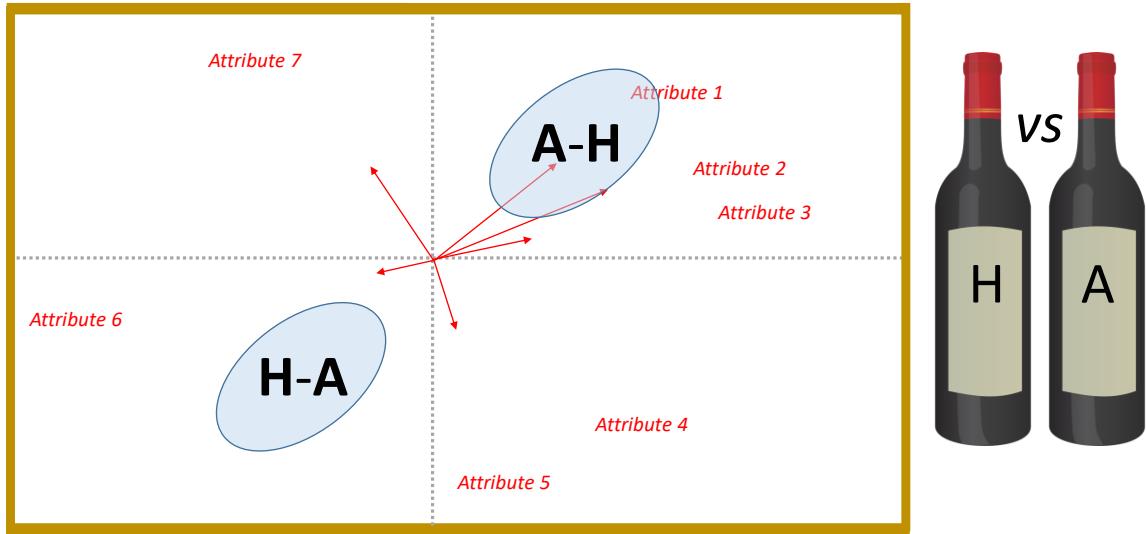
Castura, J.C., Varela, P, & Næs, T. (2023). Evaluation of complementary numerical and visual approaches for investigating pairwise comparisons after principal component analysis. *Food Quality and Preference*, 107, 104843. <https://doi.org/10.1016/j.foodqual.2023.104843>

...complementary numerical and visual approaches...

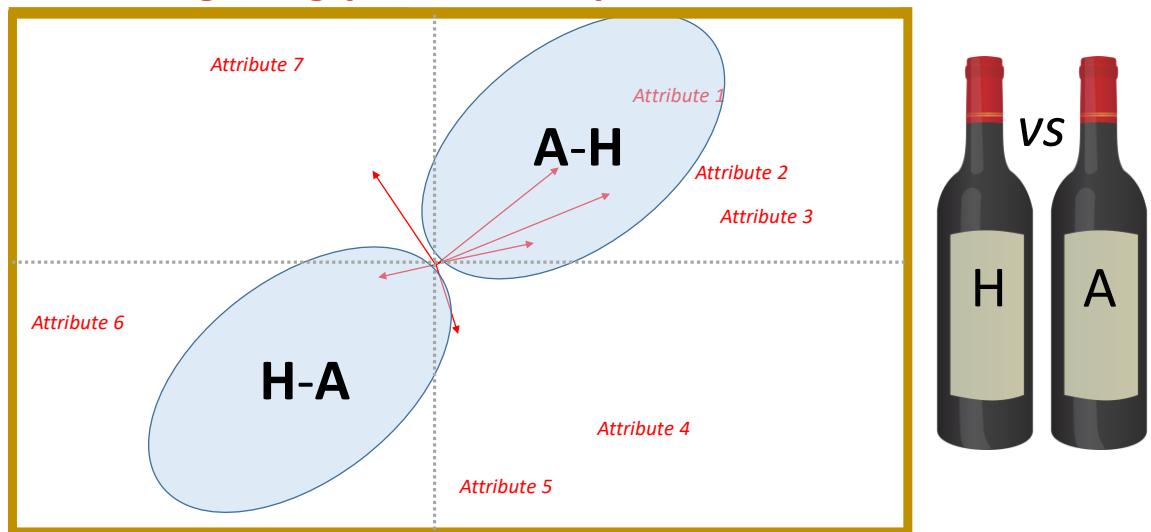
Suppl. Fig. 1a from Castura, Varela & Næs (2023a)



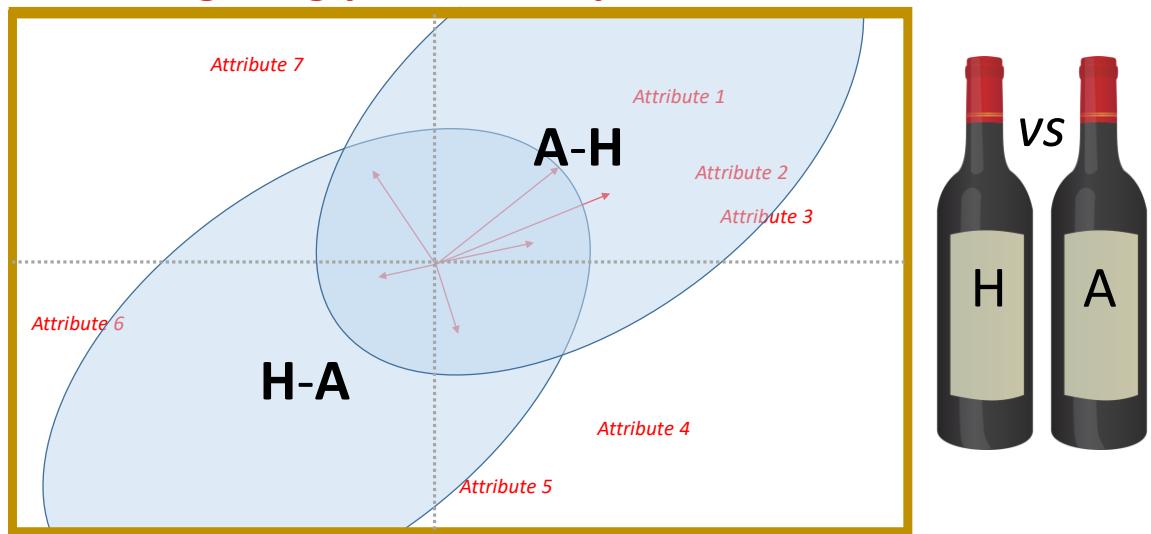
Investigating paired comparisons



Investigating paired comparisons



Investigating paired comparisons



In some studies, only a subset of paired comparisons is of primary interest...

Investigating only a subset of paired comparisons after principal component analysis

Castura, J.C., Varela, P., & Næs, T. (2023).
Investigating only a subset of paired comparisons after principal component analysis. *Food Quality and Preference*, 110, 104941.
<https://doi.org/10.1016/j.foodqual.2023.104941>

Investigating a subset of paired comparisons after PCA

Example where only a subset of paired comparisons are of primary interest:

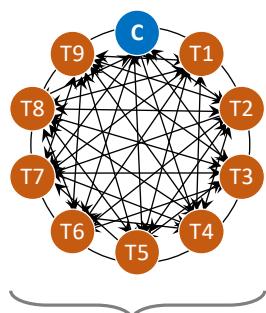
Many Test Products vs One Control

Focus on Test-Control pairs ...*not Test-Test pairs*

1 Control vs 9 Test Products

 $\times \ominus$

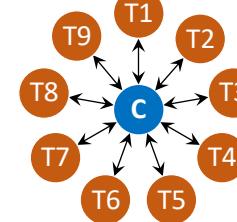
All Pairs



45 paired comparisons
90 paired differences

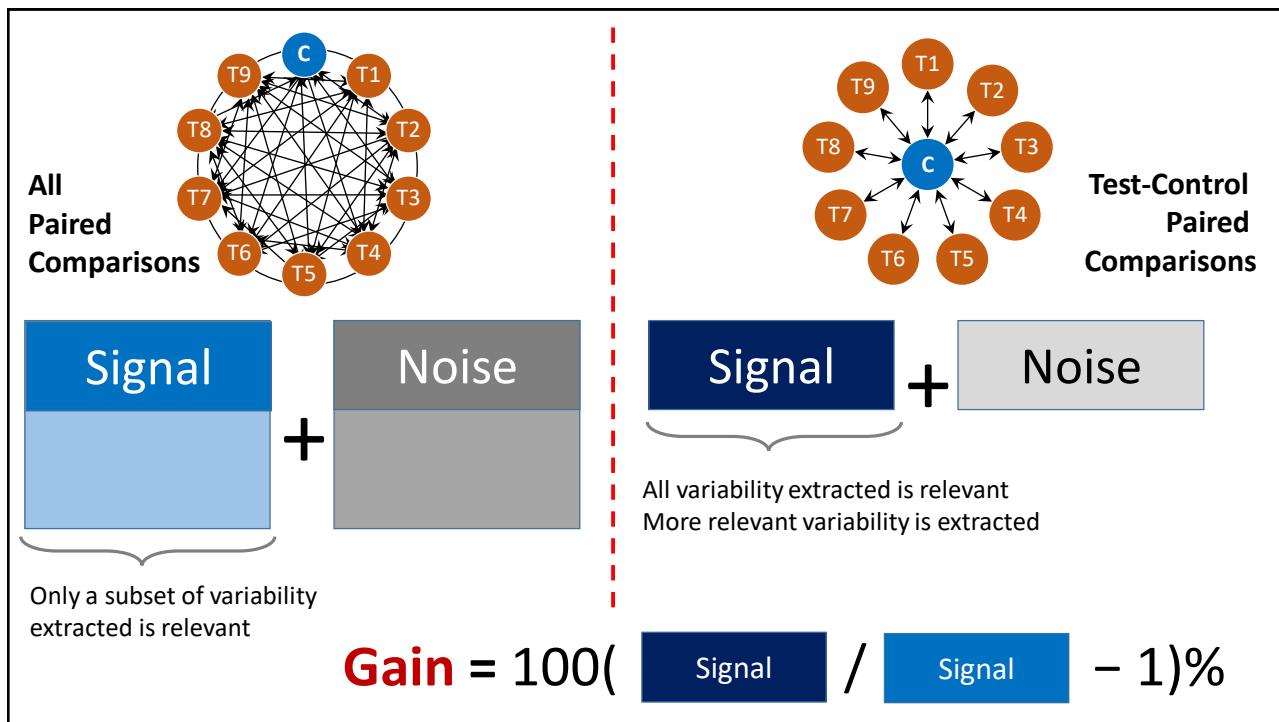
 Δ^*

Test-Control Pairs



9 paired comparisons
18 paired differences

Castura, Cariou & Næs (2024)

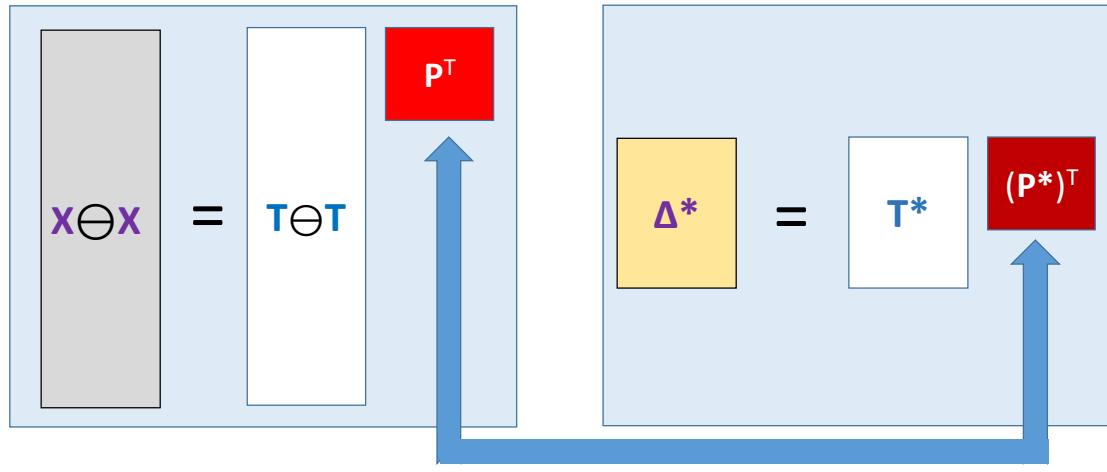


Investigating only a subset of paired comparisons

“...the interrelationships between the variables might be different for the subset of paired comparisons than it is for all paired comparisons. So the covariance matrix for a matrix of all paired comparisons and the covariance matrix of selected paired comparisons will differ depending on the data. ”

Castura, J.C., Varela, P., & Næs, T. (2023). Investigating only a subset of paired comparisons after principal component analysis. *Food Quality and Preference*, 110, 104941.

Investigating a subset of paired comparisons after PCA

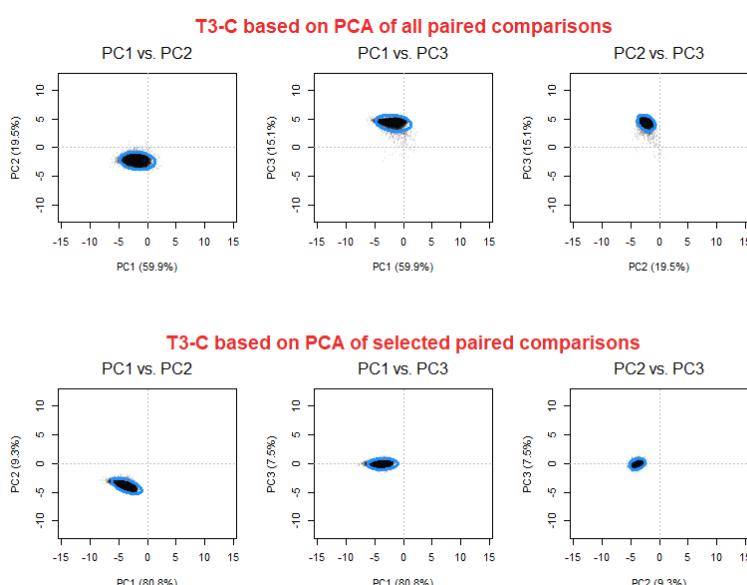


Δ^* contains a subset of the rows in $X \ominus X$

Loading matrices differ

Investigating a subset of paired comparisons after PCA

Castura, Varela, & Næs (2023) [eComponent]
doi:10.1016/j.foodqual.2023.104941



Gain:

1 PC:
15%

2 PCs:
14%

3 PCs:
1%

Investigating a subset of paired comparisons after PCA

Another example where only a subset of paired comparisons are of primary interest:

Temporal sensory data

Focus:

Paired comparisons *within* timepoints, not *across* timepoints

Investigating a subset of paired comparisons after PCA

All Pairs

- 8 yogurts \times 56 timepoints
- 448 combinations
- All pairs = 100,028

Within-timepoint Pairs

- 28 within-timepoint pairs
- 56 timepoints
- $C = 28 \times 56 = 1568$

$X \ominus X$ has dimension

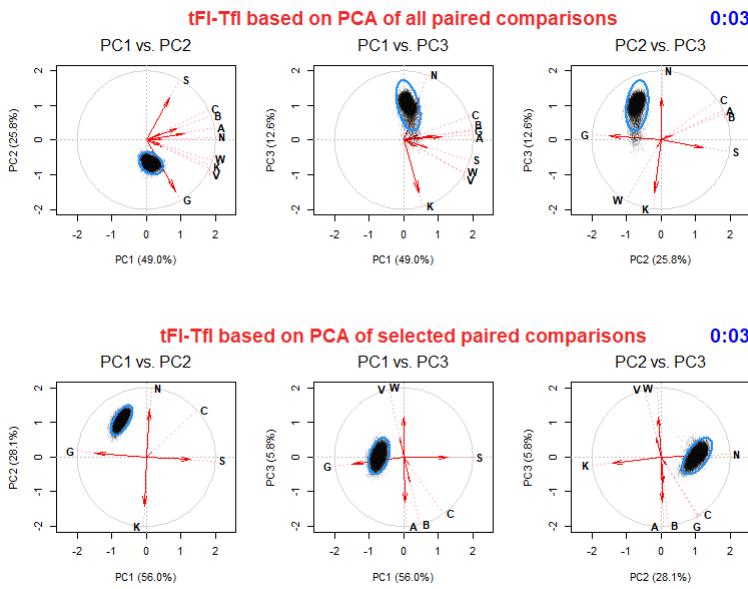
100028×10

Δ^* matrix has dimension

3136×10

Investigating a subset of paired comparisons after PCA

Castura, Varela, & Næs (2023) [eComponent]
doi:10.1016/j.foodqual.2023.104941



Gain:

1 PC: **>3500%**

2 PCs: **52%**

3 PCs: **1%**

Investigating control-centred results after uncentred principal component analysis

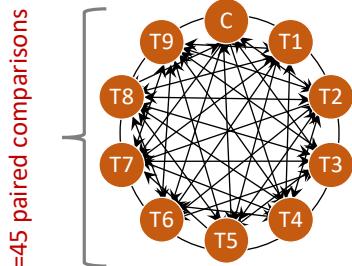
Castura, J.C., Cariou, V., & Næs, T. (2025). Investigating control-centred results after uncentred principal component analysis. *Zenodo*. Preprint.
[Manuscript under review. Preprint not peer reviewed.]

This preprint to be updated very soon!

<https://doi.org/10.5281/zenodo.15073361>

1 Control & 9 Test Products

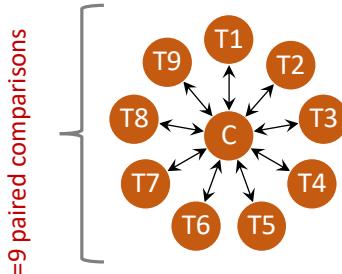
All Pairs



$$\mathbf{X} \ominus \mathbf{X}$$

$$J^2 = 100 \text{ rows}$$

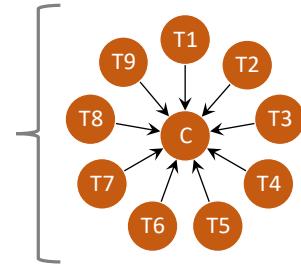
Test-Control Pairs



$$\Delta^*$$

$$2C=18 \text{ rows}$$

Test-Control Differences

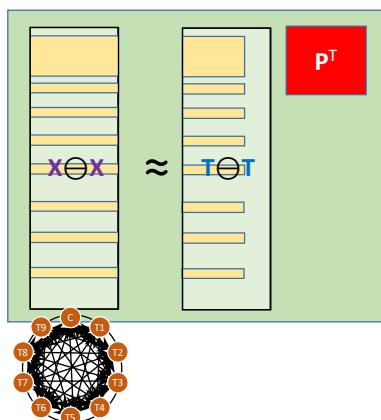


$$\mathbf{X}^c$$

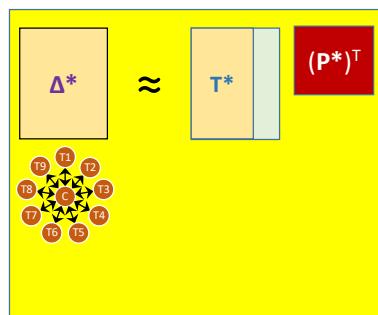
$$C+1=10 \text{ rows}$$

Castura, Cariou & Næs (2025)

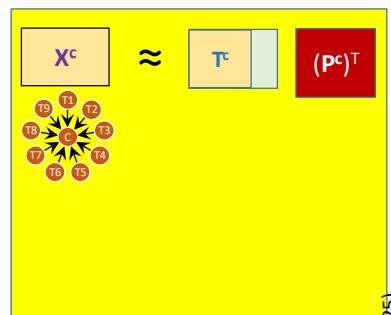
Centred PCA of $\mathbf{X} \ominus \mathbf{X}$



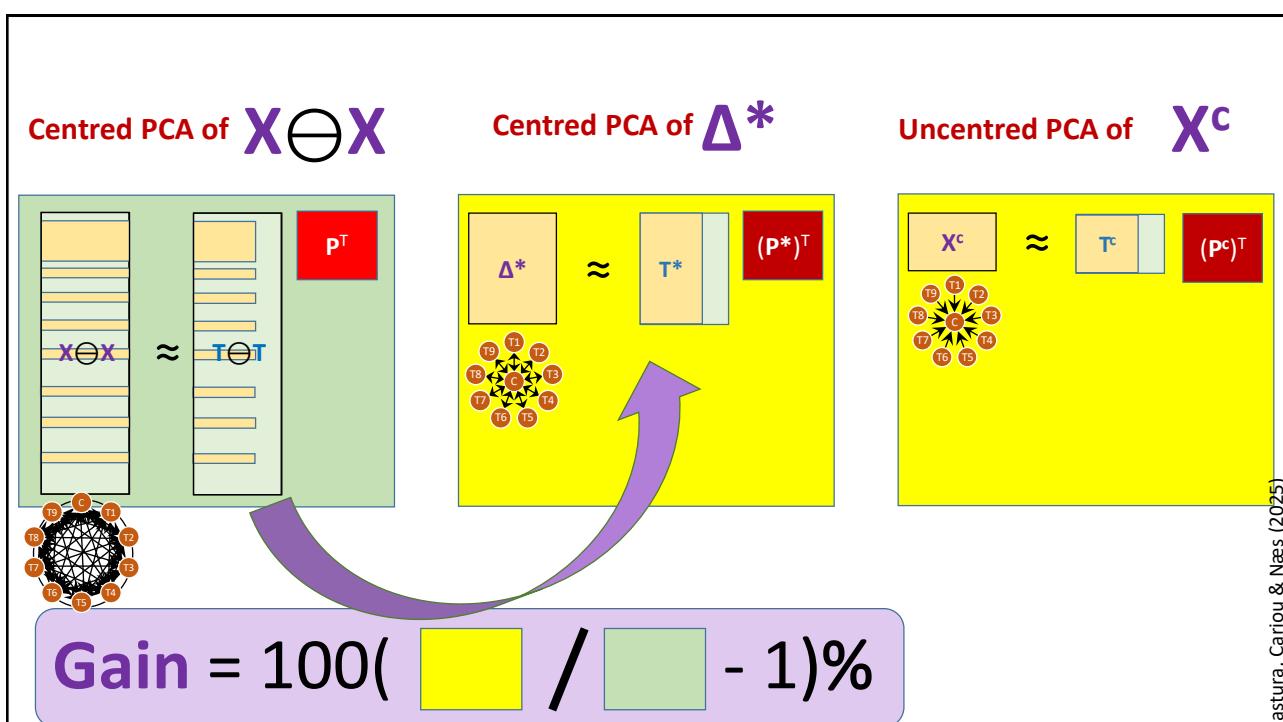
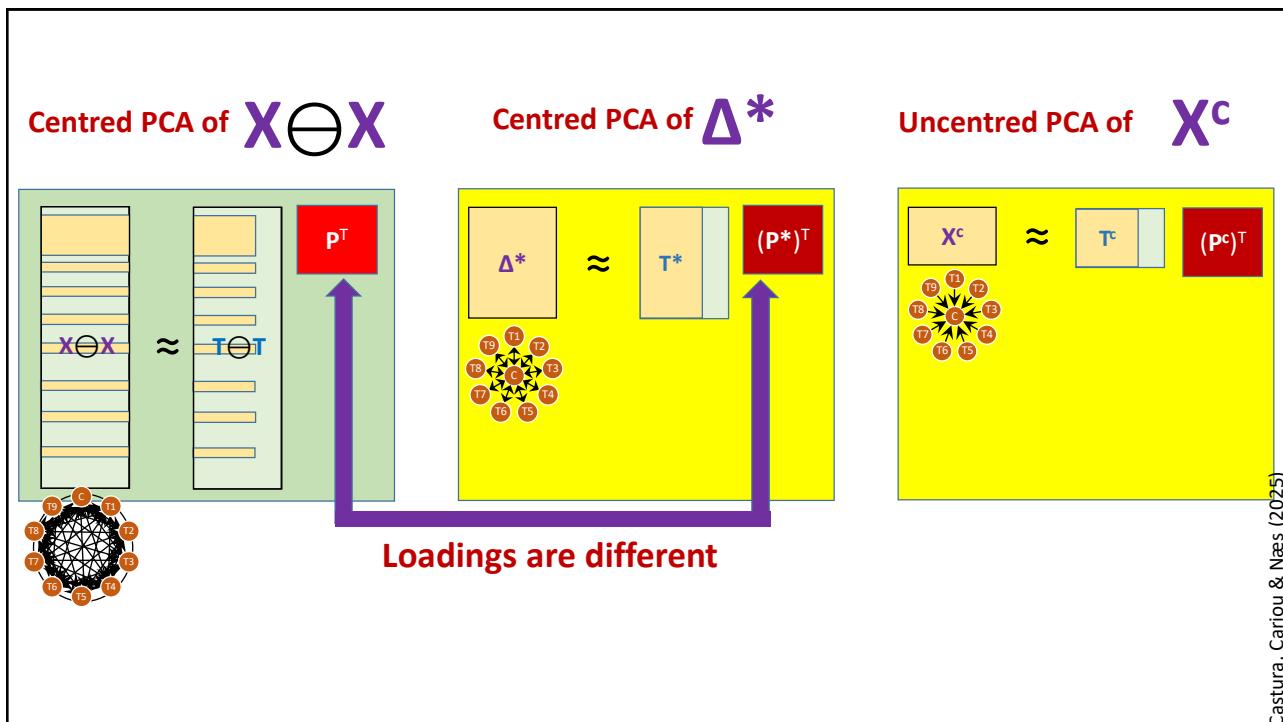
Centred PCA of Δ^*

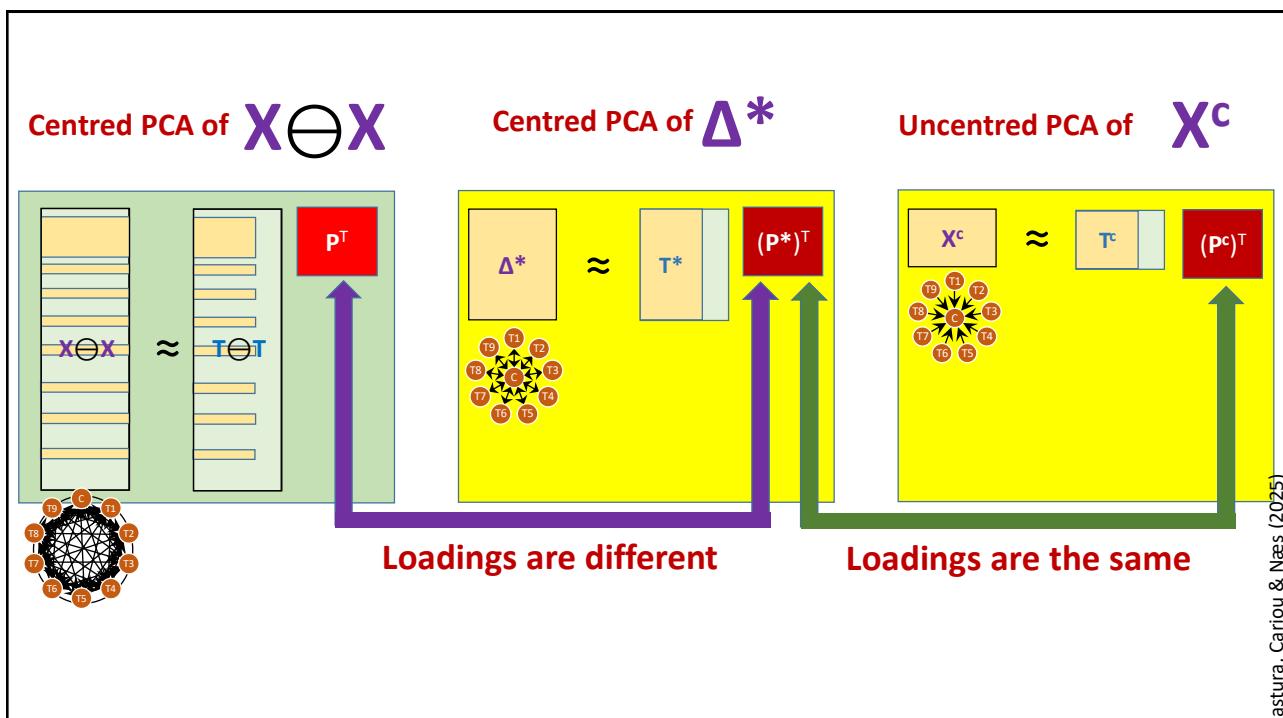
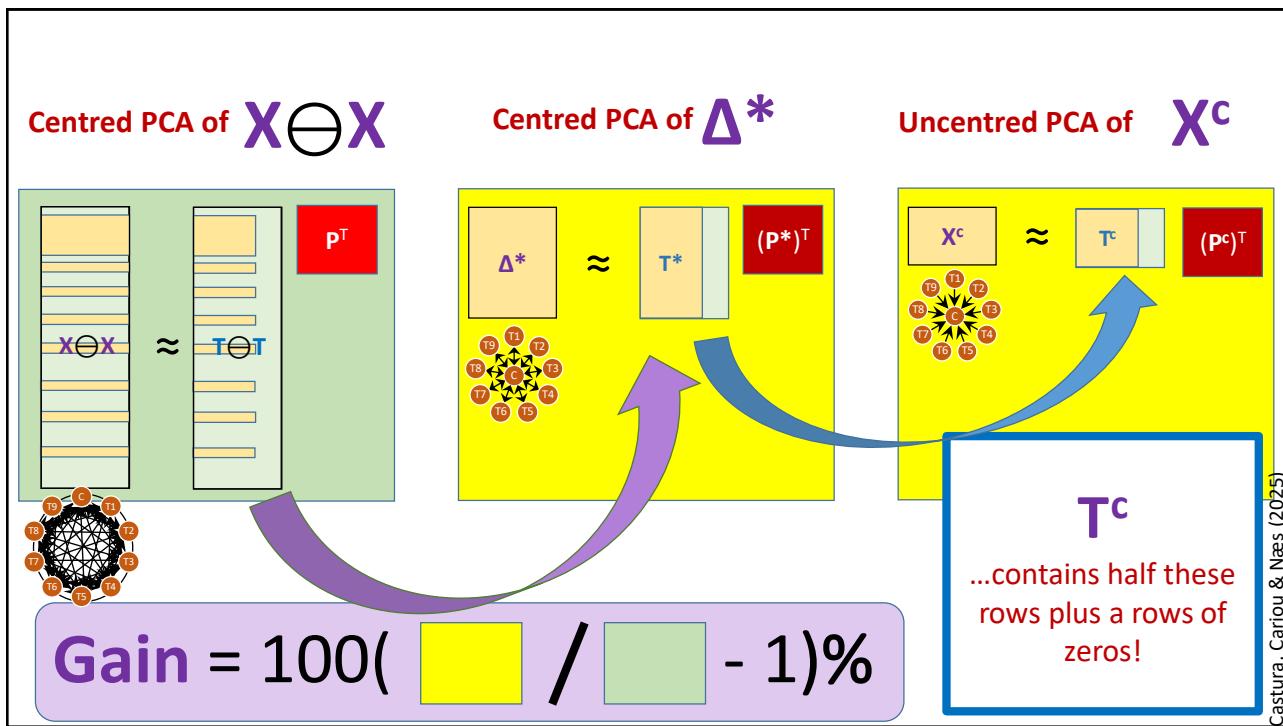


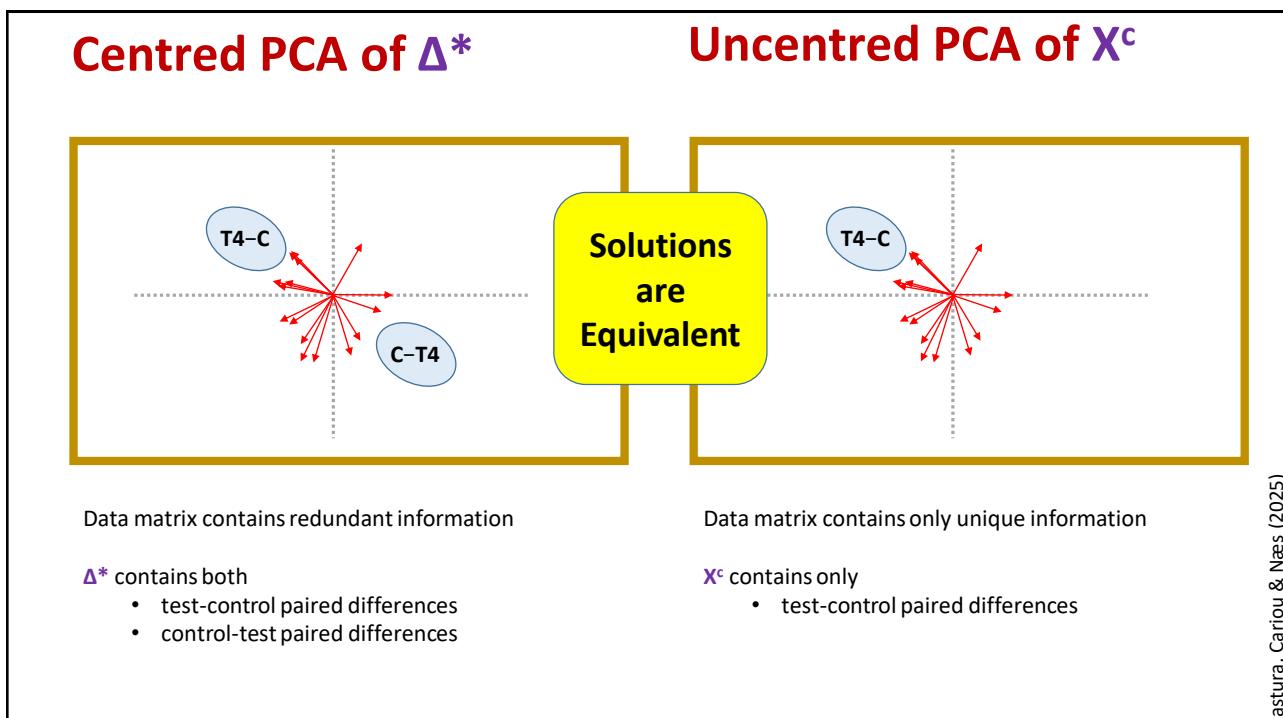
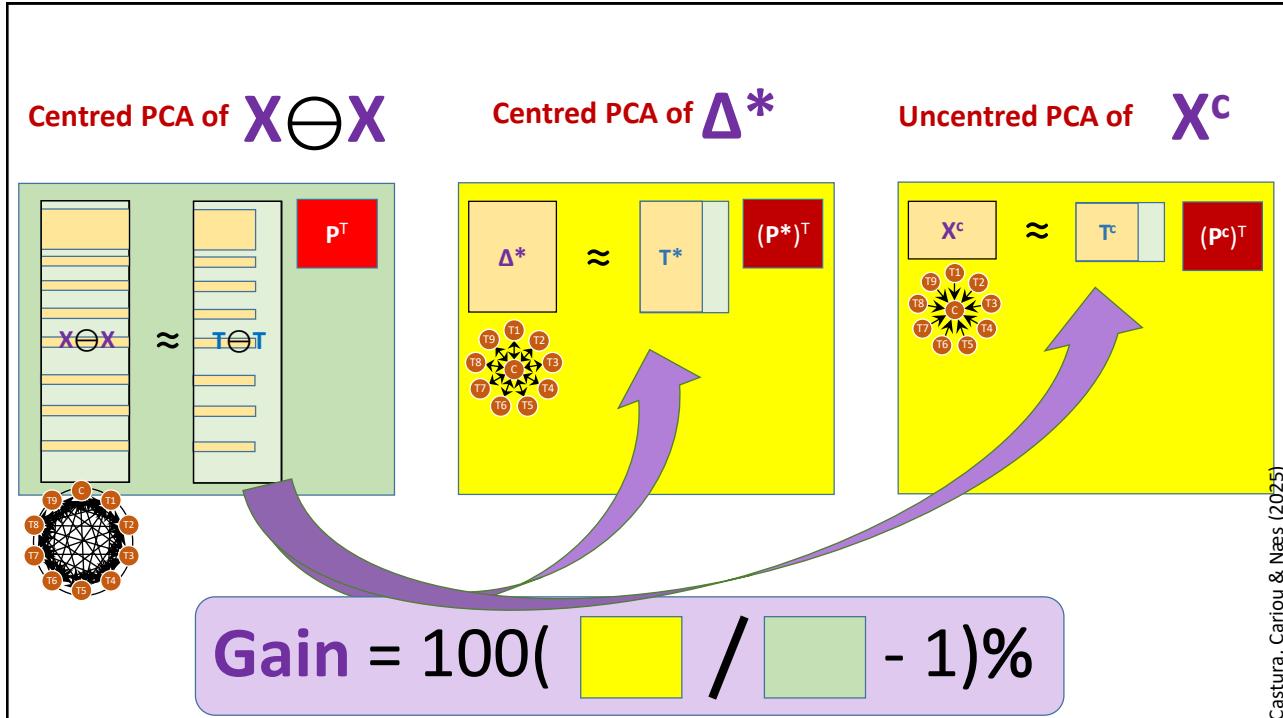
Uncentred PCA of \mathbf{X}^c



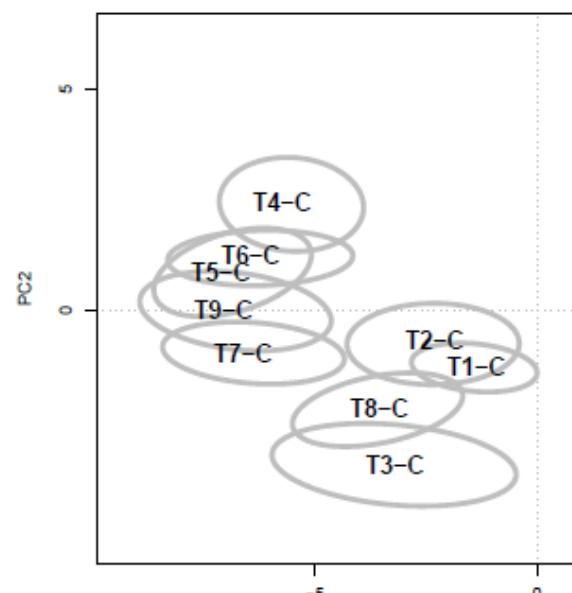
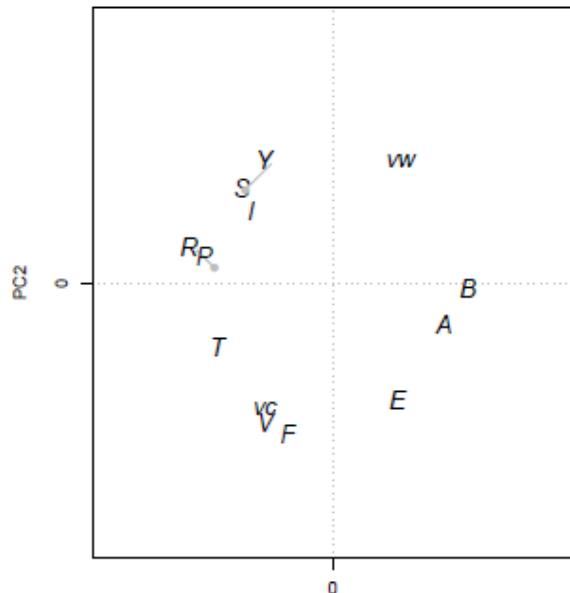
Castura, Cariou & Næs (2025)





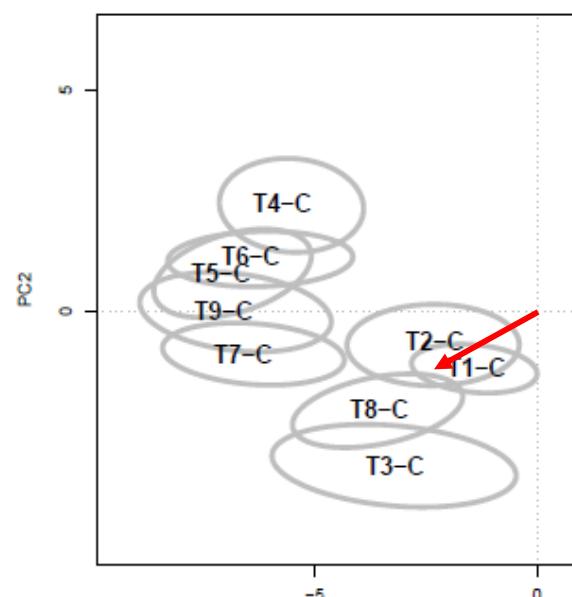
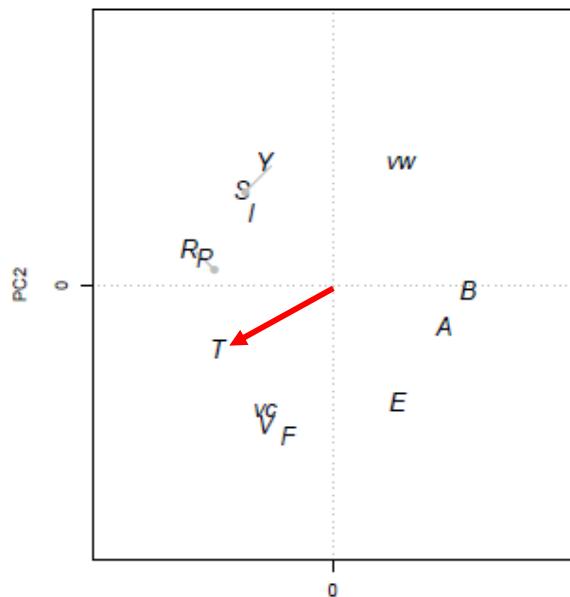


Uncentred PCA of X^c



Castura, Cariou & Næs (2025)

Uncentred PCA of X^c



Castura, Cariou & Næs (2025)

For investigating Test-Control paired comparisons...

Advantages of uncentred PCA of X^c

- “best” subspace for investigating the relevant test-control pairs
- components ordered by importance
- these particular uncentred PCA results have a conventional “variance interpretation”
- origin interpretation: “no difference from control”

Supervised principal component regression of selected paired comparisons

Castura, J.C., & Tomic, O. (2024). Supervised principal component regression of select paired comparisons. *Zenodo*. [Manuscript under review. Preprint not peer reviewed].

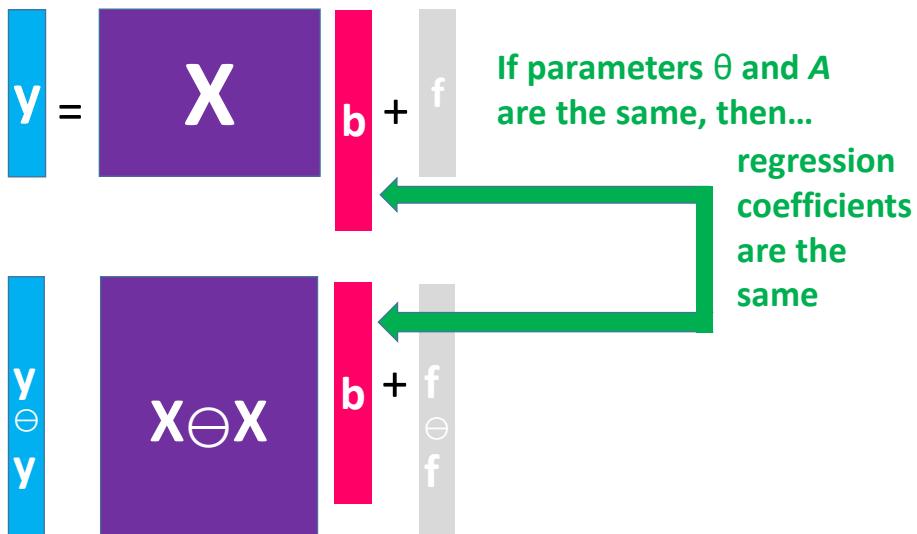
<https://doi.org/10.5281/zenodo.11663995>

This preprint to be updated very soon!

Castura, J.C., & Tomic, O. (2025). Supervised principal component regression of select paired comparisons. [To be uploaded soon to the *Zenodo* preprint server!] [Manuscript under review. Preprint not peer reviewed].

Investigating data relationships

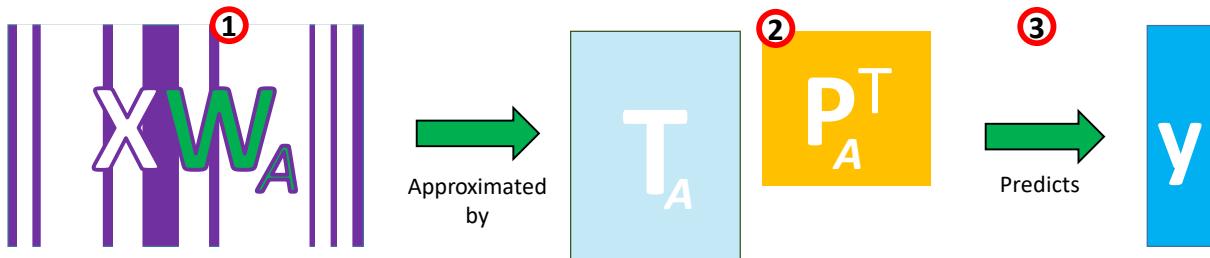
with **supervised principal component regression (SPCR)**



Castura & Tomic (2024)

Investigating data relationships

with **supervised principal component regression (SPCR)**



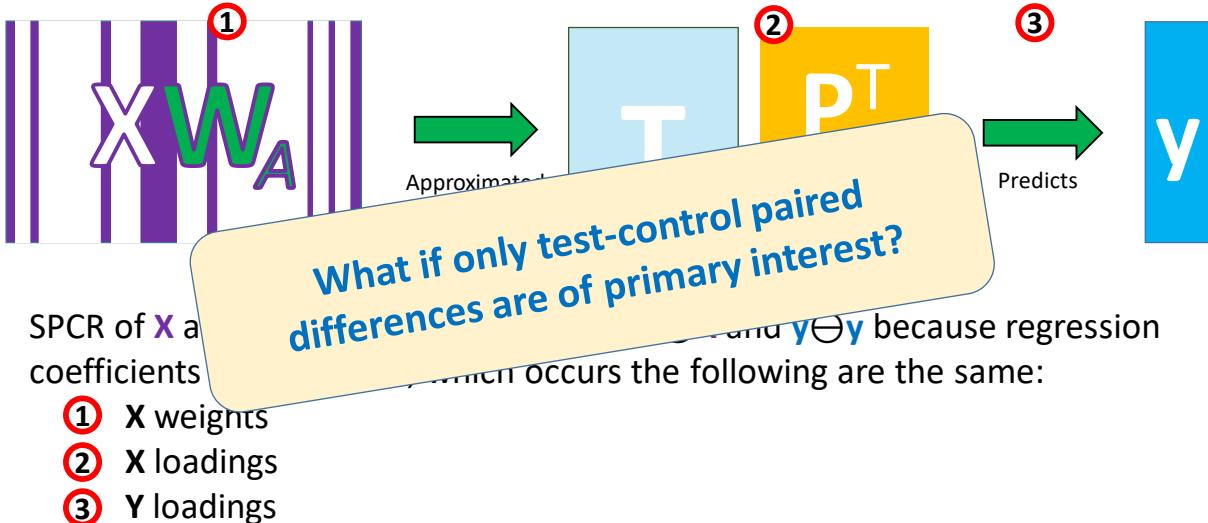
SPCR of X and y is equivalent to SPCR of $X \ominus X$ and $y \ominus y$ because regression coefficients are the same, which occurs when the following are the same:

- ① X weights
- ② X loadings
- ③ Y loadings

Castura & Tomic (2024)

Investigating data relationships

with **supervised principal component regression (SPCR)**



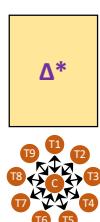
Castura & Tomic (2024)

Investigating data relationships

with **supervised principal component regression (SPCR)**

We know we can focus on paired comparisons or paired differences since...

Centred PCA of Δ^*

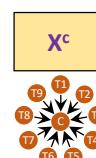


\approx



...is equivalent to...

Uncentred PCA of X^c



\approx

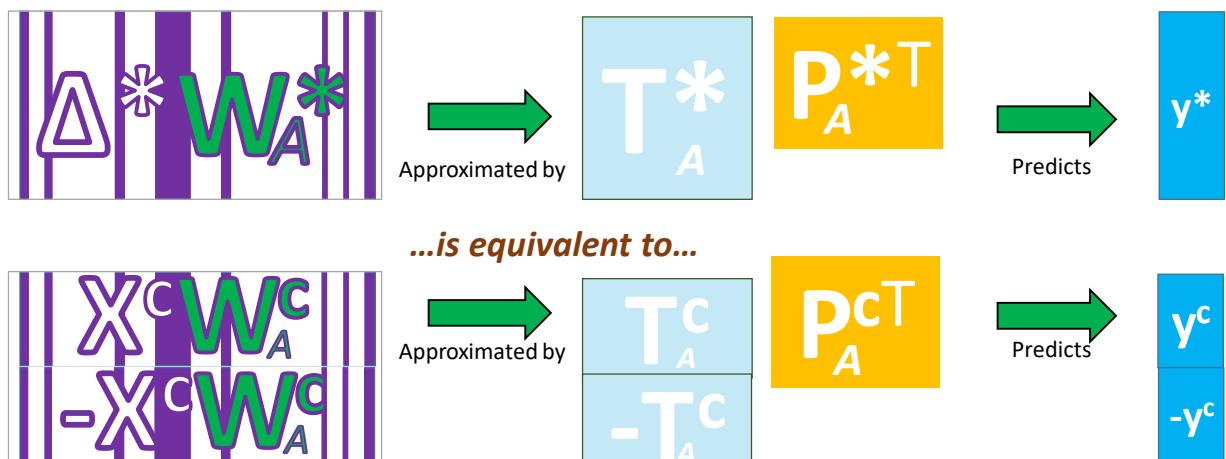


...however, using Δ^* introduces a subtle problem...

Castura & Tomic (2025)

Investigating data relationships

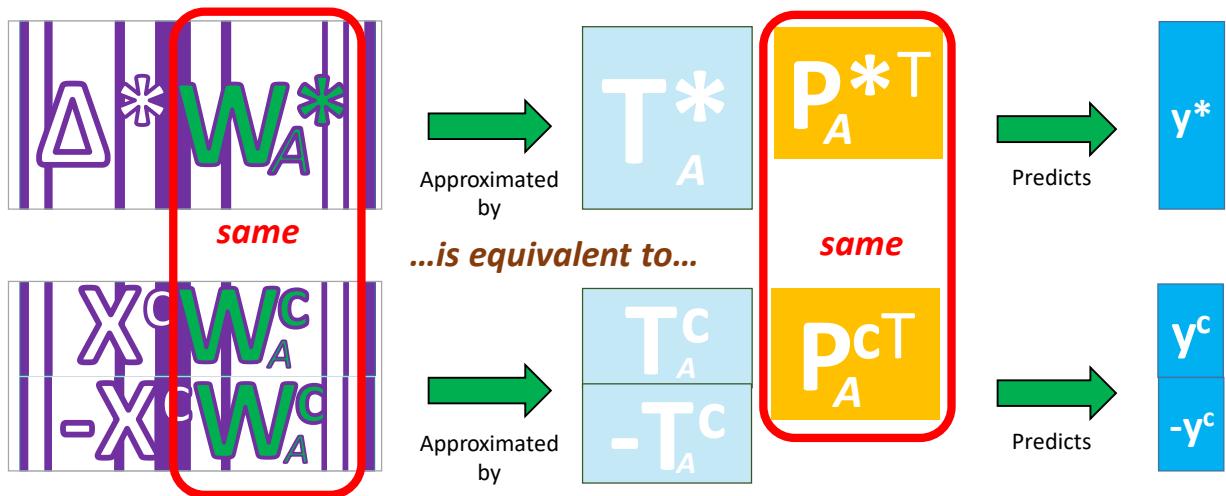
with supervised principal component regression (SPCR)



Castura & Tomic (2025)

Investigating data relationships

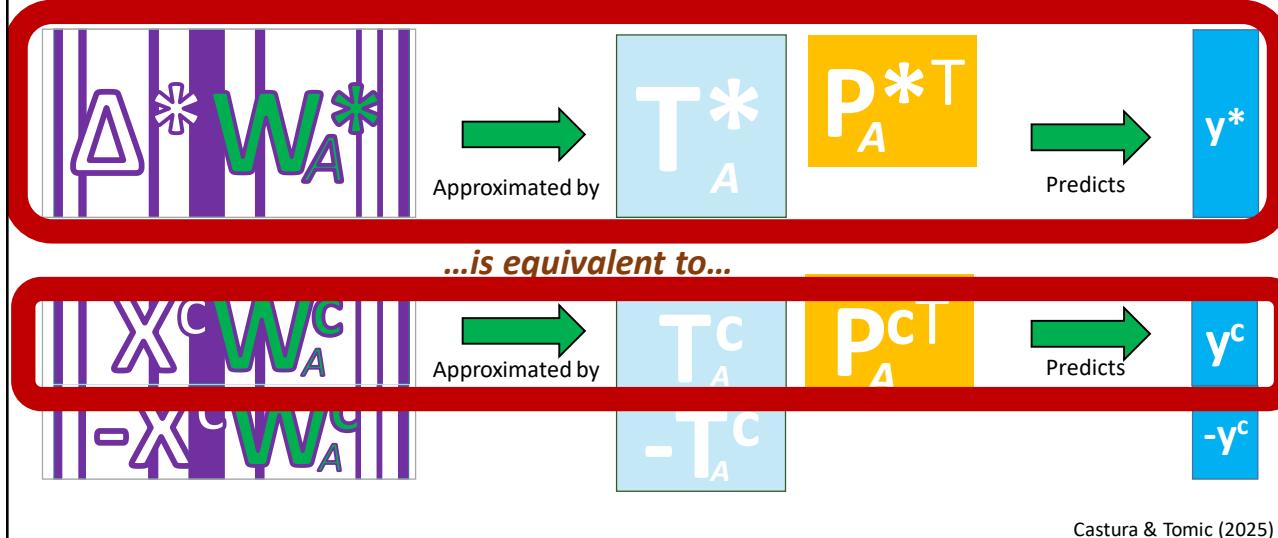
with supervised principal component regression (SPCR)



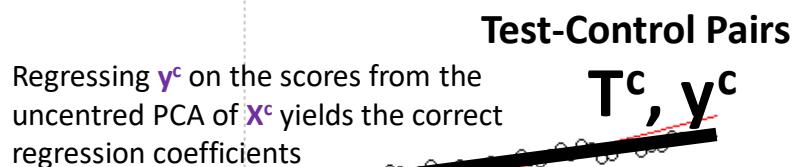
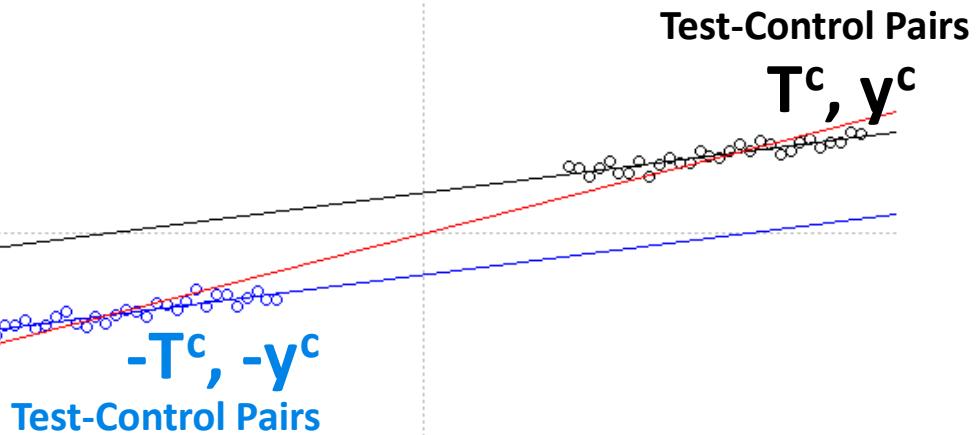
Castura & Tomic (2025)

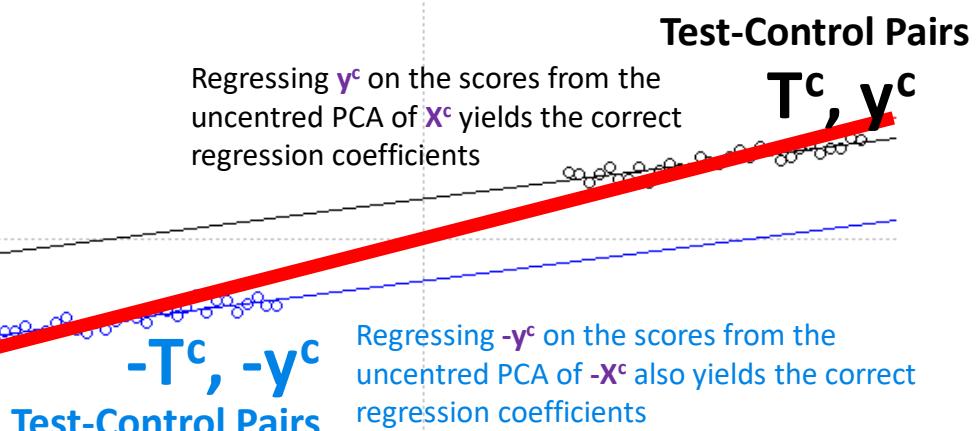
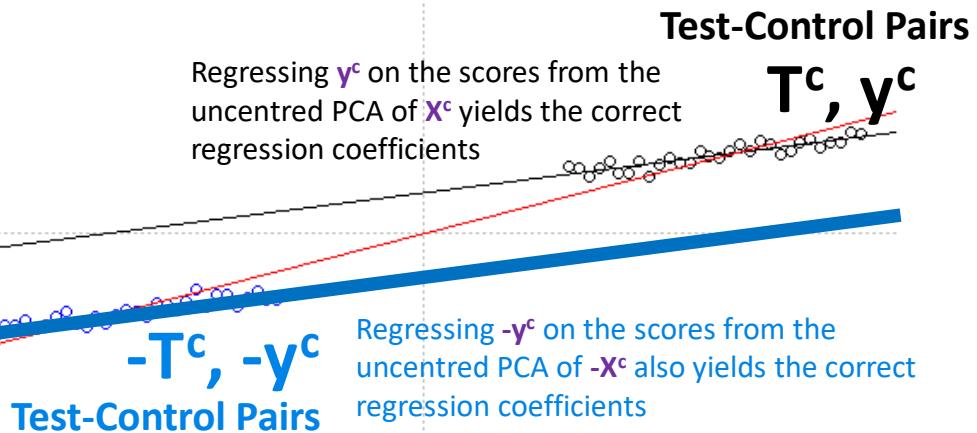
Investigating data relationships

with supervised principal component regression (SPCR)



...however, using Δ^* introduces a subtle problem...





Both Test-Control Pairs & Control-Test Pairs

Regressing $y^* = (y^c, -y^c)$ on the scores from the uncentred PCA of $\Delta^* = (X^c, -X^c)$ forces the regression through the origin, leading to bad predictions!

Many candidate values for parameters θ and A

Since we are focused on paired comparisons, we **adapted leave-one-out cross-validation** to handle ***dependent data***.

Castura & Tomic (2025)

Conventional loocv

One row left out per fold.

Each row is an object.

No information from the left-out object leaks into the model during training.

Software for conventional loocv widely available.

Adapted loocv

One object left out per fold.

Multiple rows are left out.

No information from the left-out object can leak into the model during training.

Functions for adapted loocv must be coded.

Castura & Tomic (2025)

Predicted error sum of squares (PRESS)

Models evaluated by calculating PRESS statistic calculated for left-out test-control paired differences.

$$\sum (predicted - observed)^2$$

Castura & Tomic (2025)

Investigating data relationships

with **supervised principal component regression (SPCR)**

$$\mathbf{y} = \mathbf{X} \mathbf{b} + \mathbf{f}$$

If using
loocv...

...SPCR of test-control paired
differences has different
regression coefficients

$$\mathbf{y} = \mathbf{X} \mathbf{b} + \mathbf{f} \ominus \mathbf{f}$$

...SPCR of all
objects has
the same
regression
coefficients
as SPCR of
all paired
differences

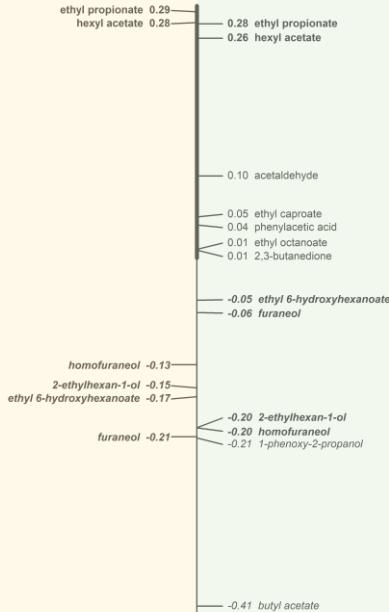
$$\mathbf{y}^c = \mathbf{X}^c \mathbf{b}^c + \mathbf{f}^c$$

Castura & Tomic (2025)

Cooked
cherry
aroma

6 Predictors
2 PCs
PRESS 1.75

Regression coefficients



SPCR of $\mathbf{X} \ominus \mathbf{X}$ and $\mathbf{y} \ominus \mathbf{y}$

13 Predictors
2 PCs
PRESS 1.48

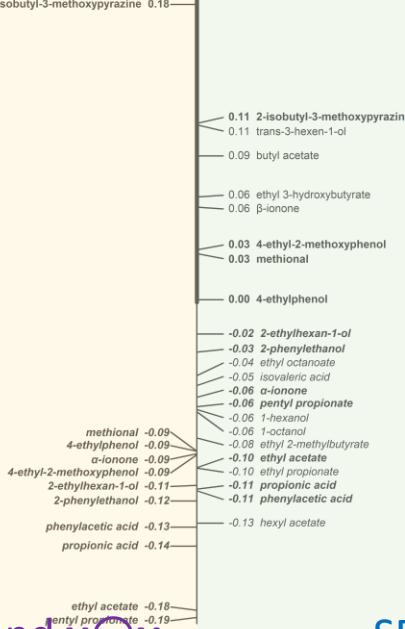
SPCR of \mathbf{X}^c and \mathbf{y}^c

Castura & Tomic (2025)

Fresh
cherry
aroma

11 Predictors
1 PCs
PRESS 1.67

Regression coefficients

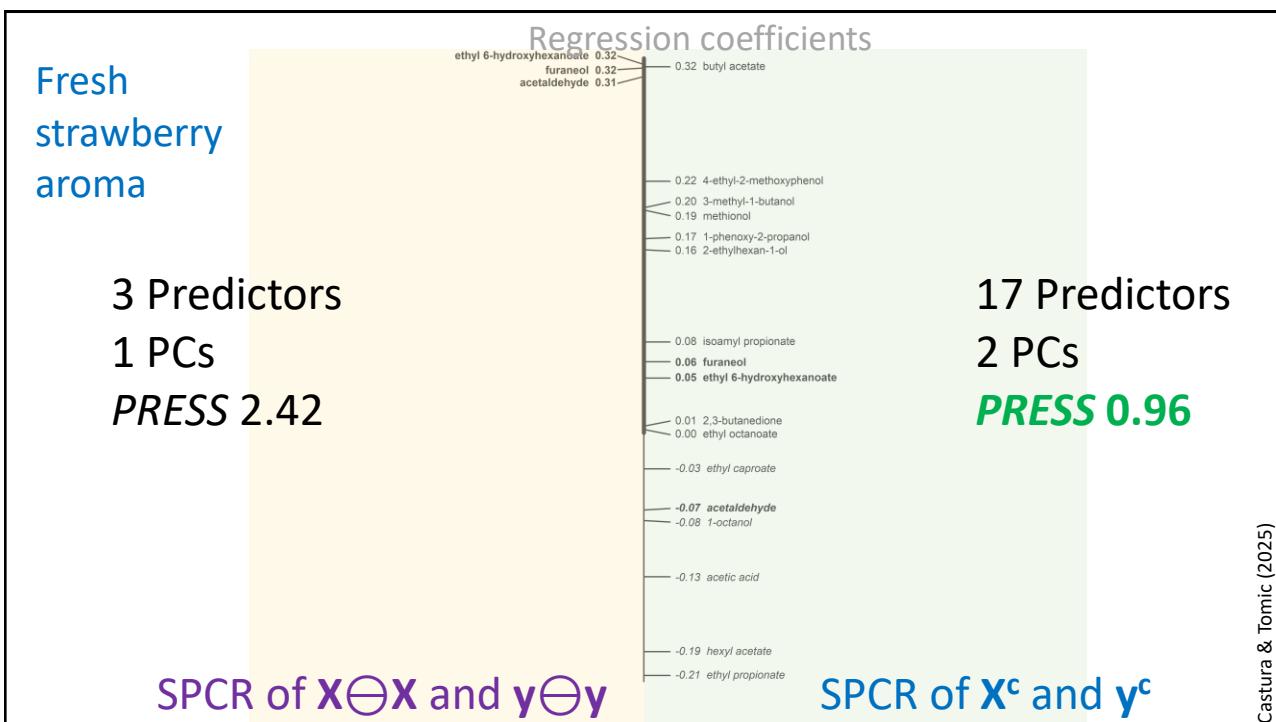
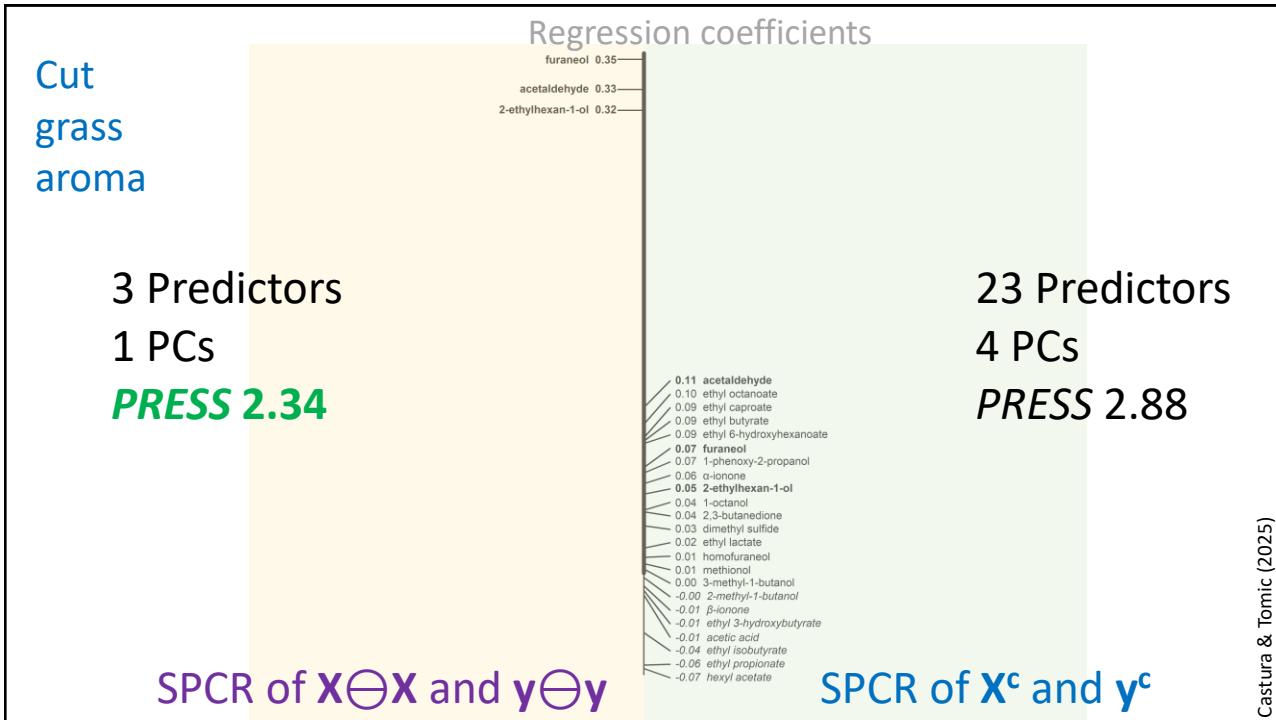


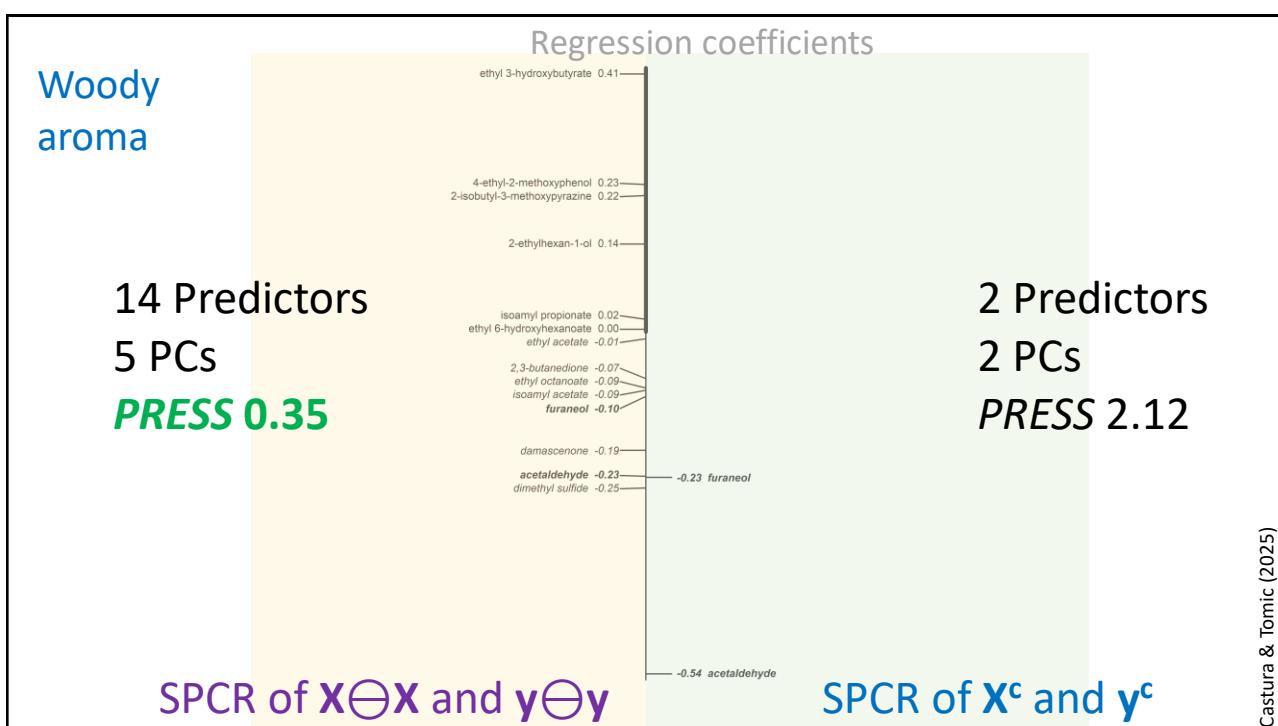
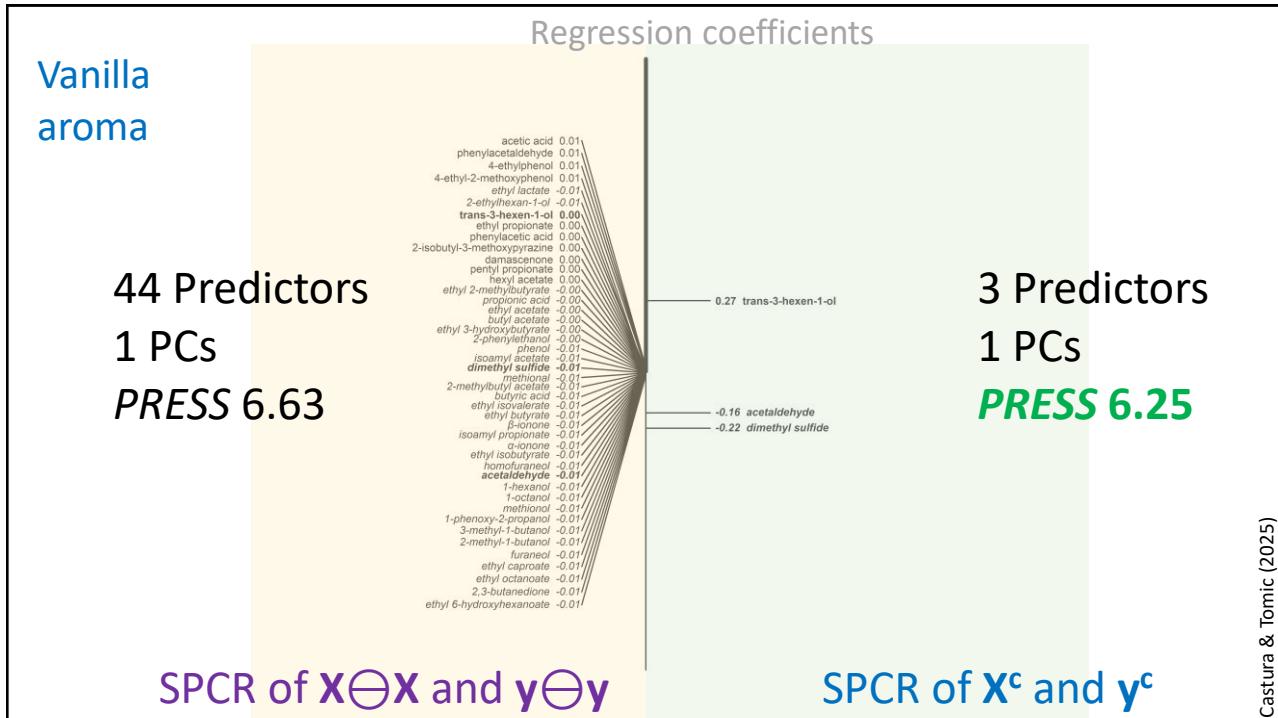
SPCR of $\mathbf{X} \ominus \mathbf{X}$ and $\mathbf{y} \ominus \mathbf{y}$

22 Predictors
3 PCs
PRESS 0.89

SPCR of \mathbf{X}^c and \mathbf{y}^c

Castura & Tomic (2025)





Simulation study

Each condition was a combination of...

Number of “signal variables”: 5, 15, 30, 45.
Std dev of random added noise: 0, $\frac{1}{4}$, $\frac{1}{2}$, $\frac{3}{4}$, 1.

simulate

3 latent
variables

project

pure signal
variables

add noise

add noise

signal noise

Training data set

simulate

signal noise

Test data set

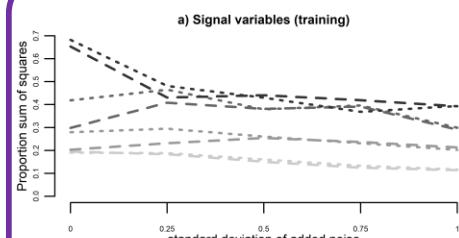
simulate

Castura & Tomic (2025)

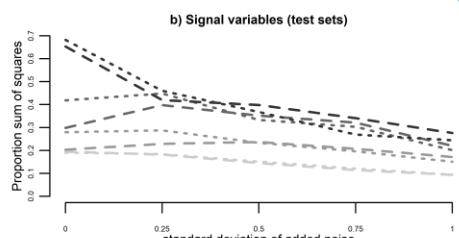
Simulation study

Results
based
on
loocv

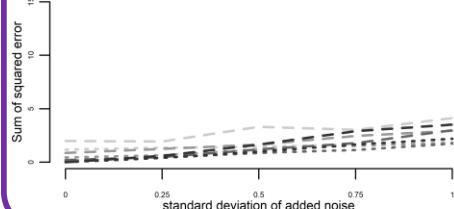
a) Signal variables (training)



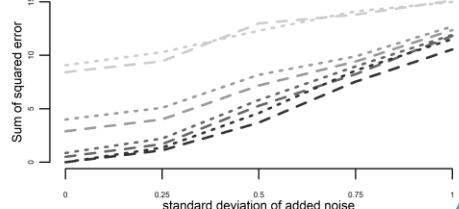
b) Signal variables (test sets)



c) Predicted responses (training)



d) Predicted responses (test sets)



Signal variables

5 15 30 45

SPCR model

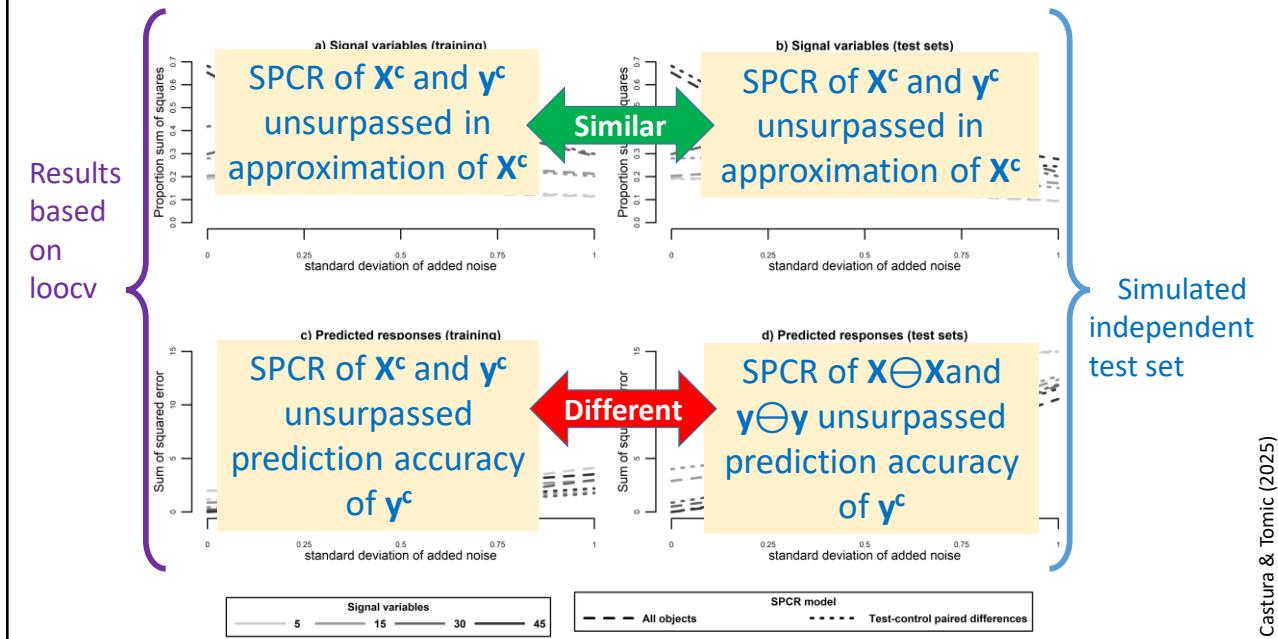
— All objects

--- Test-control paired differences

Simulated
independent
test set

Castura & Tomic (2025)

Simulation study



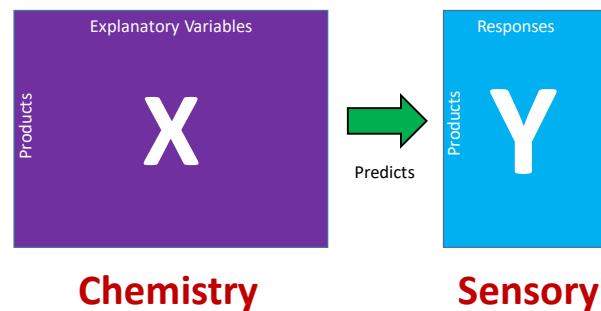
Castura & Tomic (2025)

The simulation study shows the superiority of the SPCR of test-control paired differences model for the training set does not generalize to test sets simulated from the same data generating process.

We are only interested in the test-control paired differences, not the test-test paired differences, but since both types of pairs carry information about the association between variables, the relationship between predictor and response variables is modelled better by the SPCR of all objects model than by the SPCR of test-control paired differences model.

This finding shows **overfitting appears in many guises**. For this reason, the SPCR of all objects model is recommended for most routine analyses.

Castura & Tomic (2025)



Partial least squares regression (PLSR)

Partial least squares regression (PLSR)

We want to *predict* multivariate **Y** from the multivariate **X**.

Successive PLS components extract *covariation* between **X** and **Y** maximally.

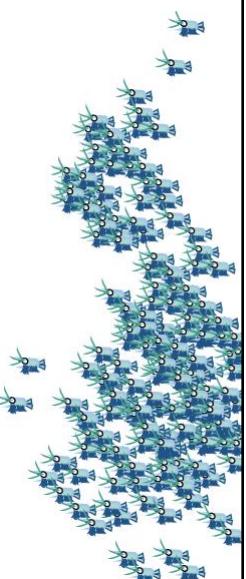
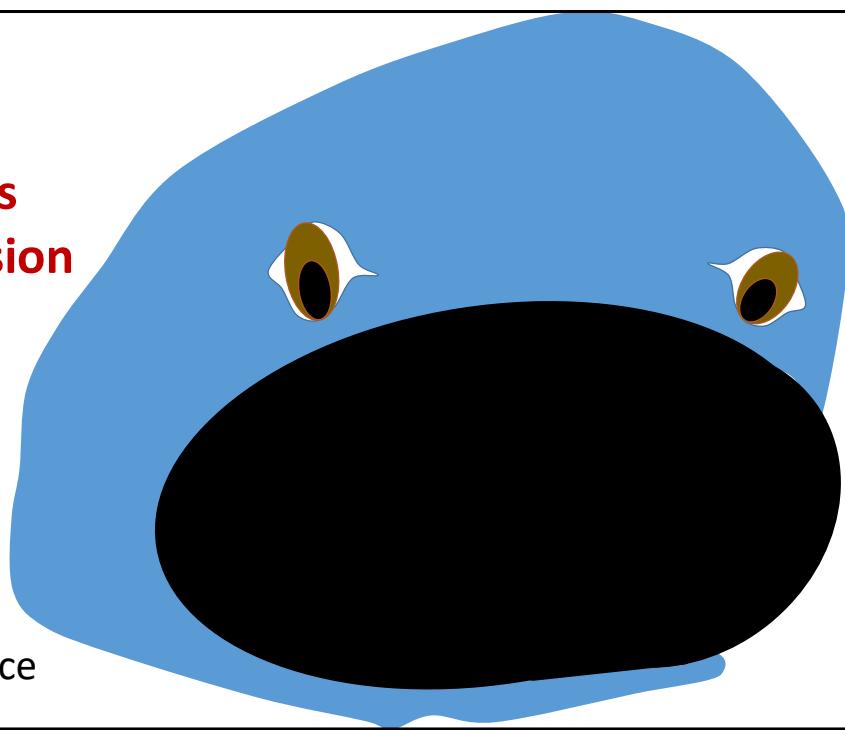
Partial least squares regression (PLSR)

We want to *predict* multivariate **Y** from the multivariate **X**.

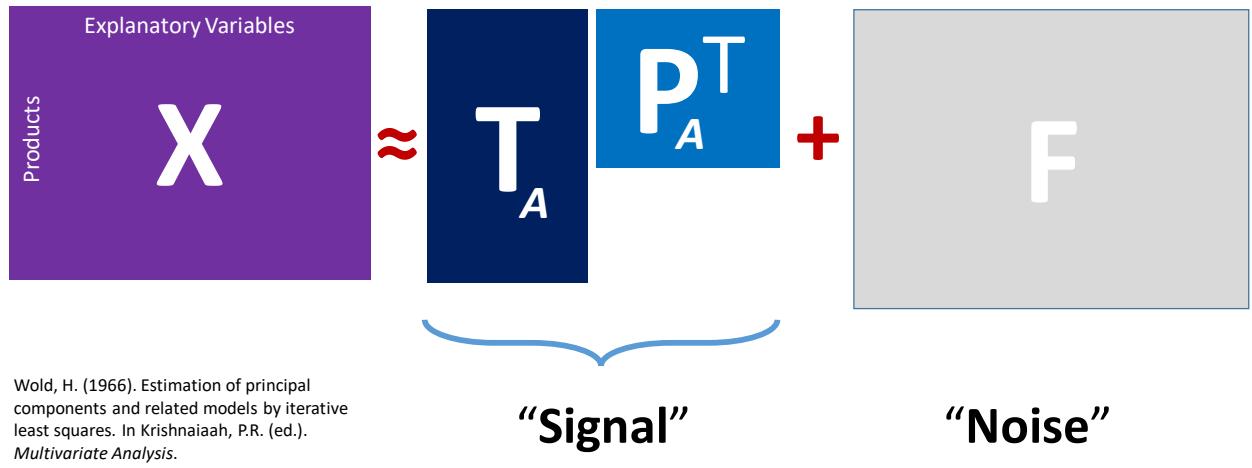
Successive **PLS components** extract *covariation* between **X** and **Y** maximally.

Partial
least
squares
regression

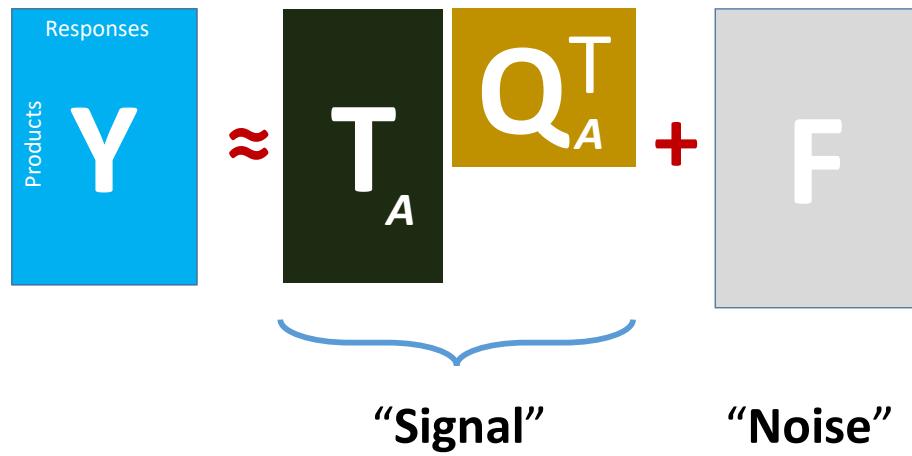
Covariance



Explaining and predicting data relationships

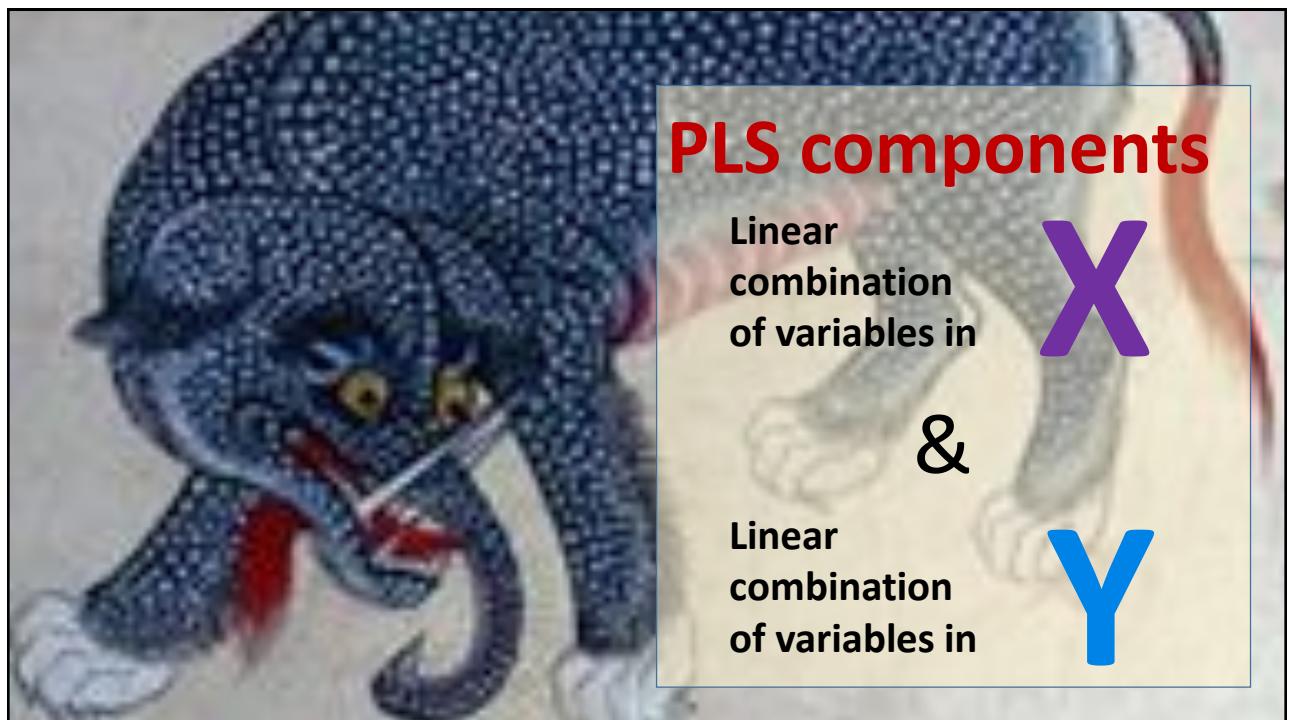
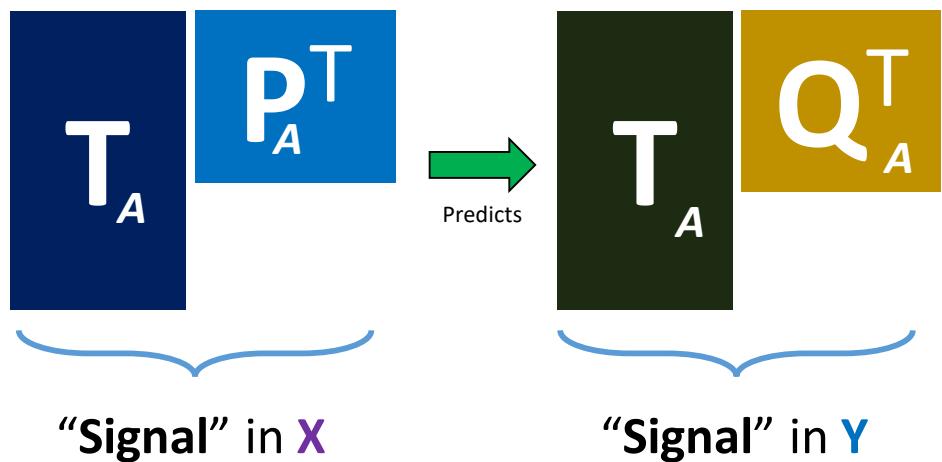


Explaining and predicting data relationships

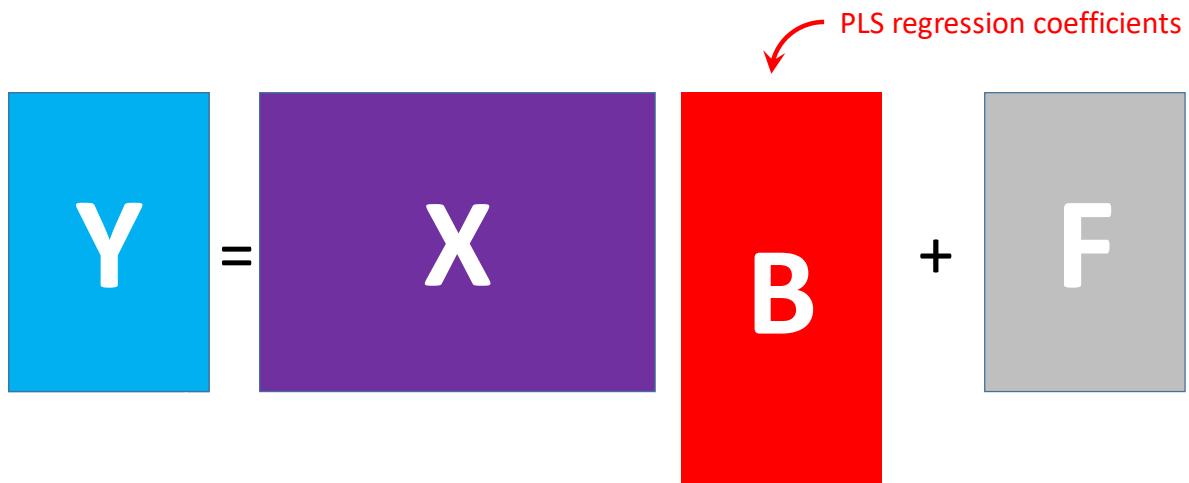


Wold (1966)

Partial least squares regression (PLSR)

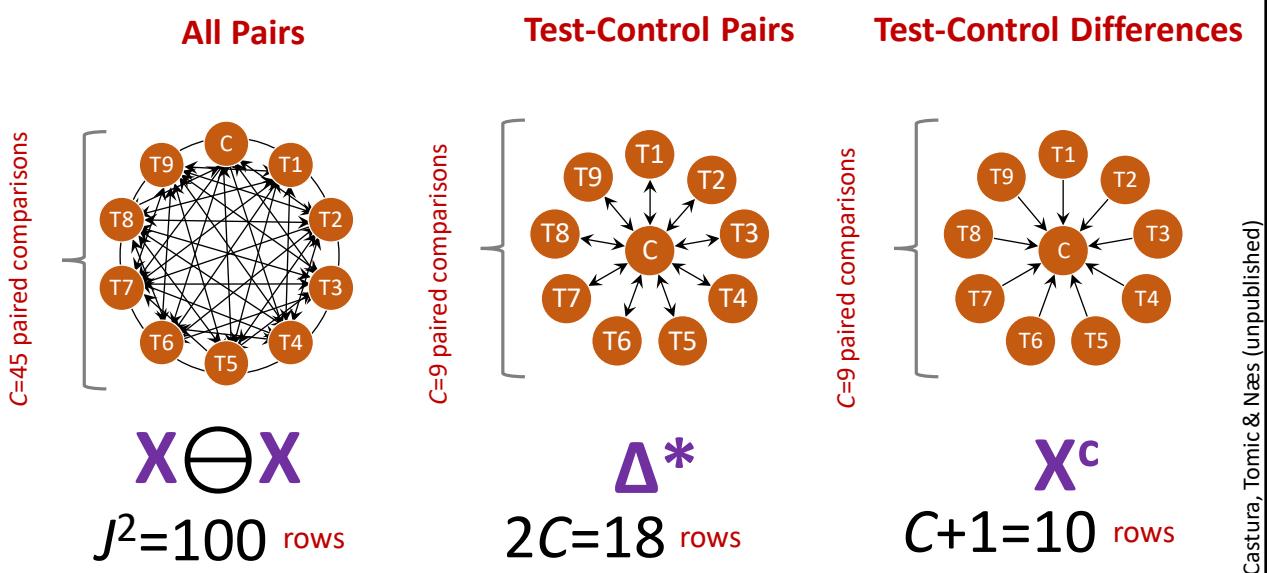


Investigating data relationships



Wold (1966)

Paired comparisons after PLSR



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John Castura



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of Life Sciences



Exploring the relationship between sensory and instrumental data with component-based methods



KoSFoST International Symposium and Annual Meeting 2025

Pioneering Future Connection in FoodTech
Gwangju, Korea · 2-4 July 2025

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