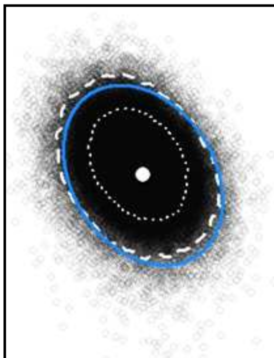


Evaluation of complementary numerical and visual approaches for investigating pairwise comparisons after principal component analysis

John Castura
Compusense Inc.
Canada

Paula Varela
Nofirma AS
Norway

Tormod Næs
Nofirma AS
Norway

16th Sensometrics meeting, **A virtual reality**

Online conference, November 15 – 17, 2022

The Sensometric Society

1. Researcher designs experiment and collects data.

2. Data analysis.

Automated data analysis.
Screening for unusual results.
Visualizations for review.

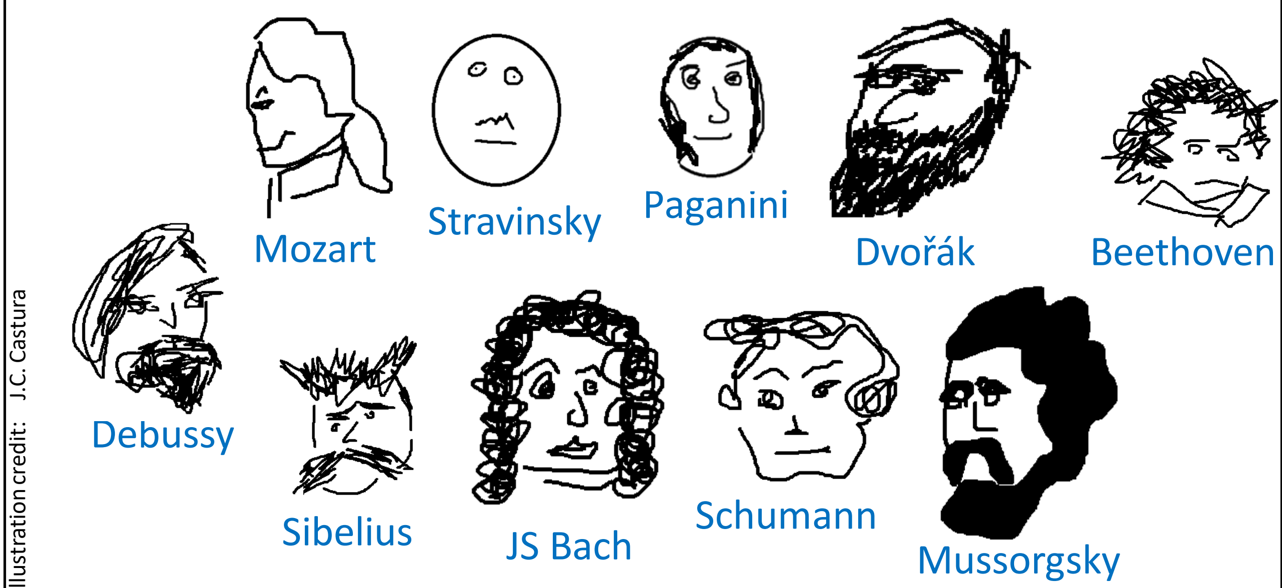
3. Interpretation of results.

4. Recommendations and decisions.

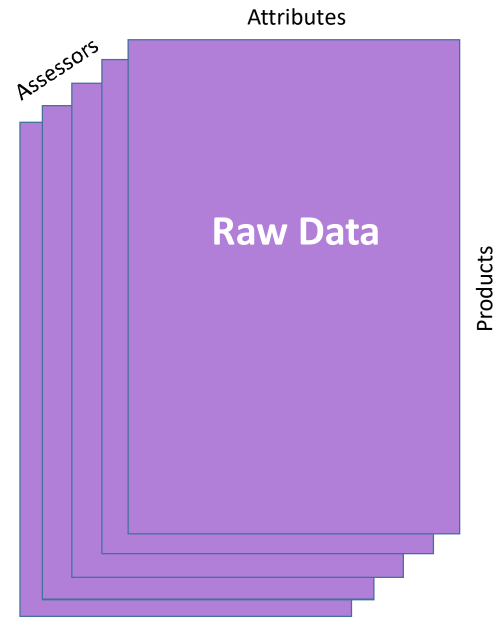
Principal Component Analysis

PCA

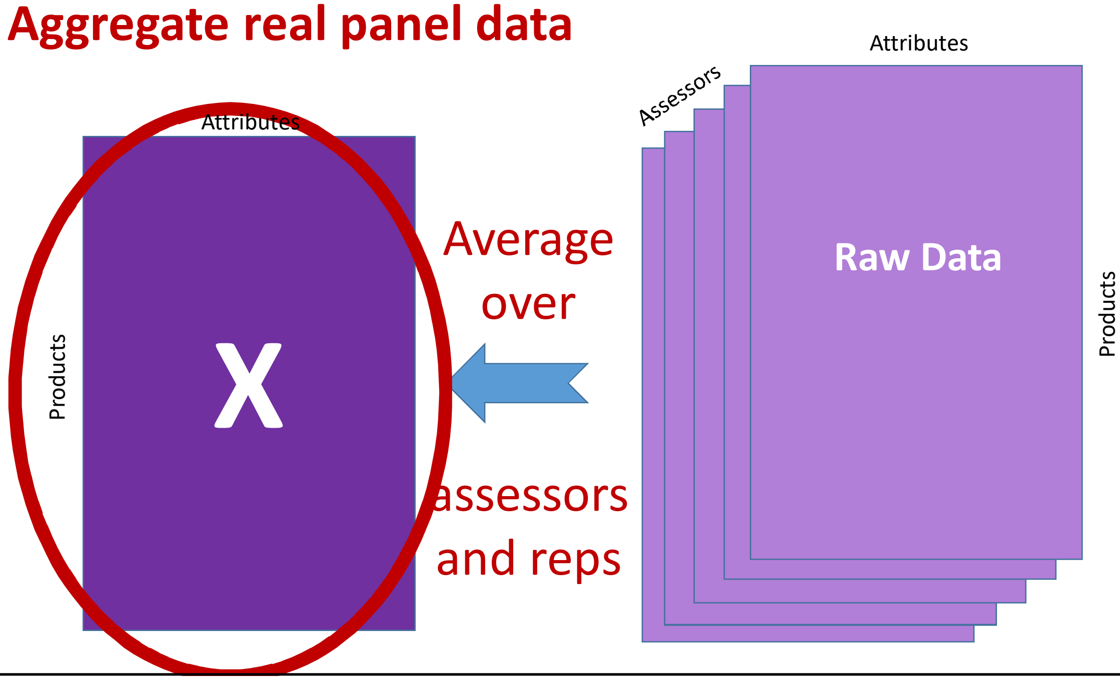
Panel of Sensory Assessors



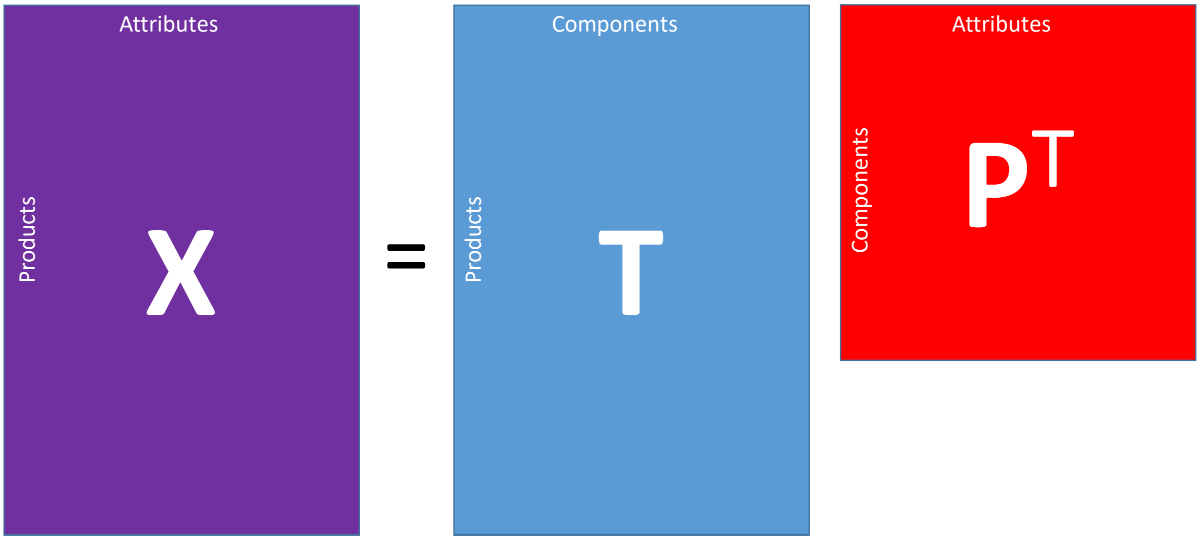
Real panel data



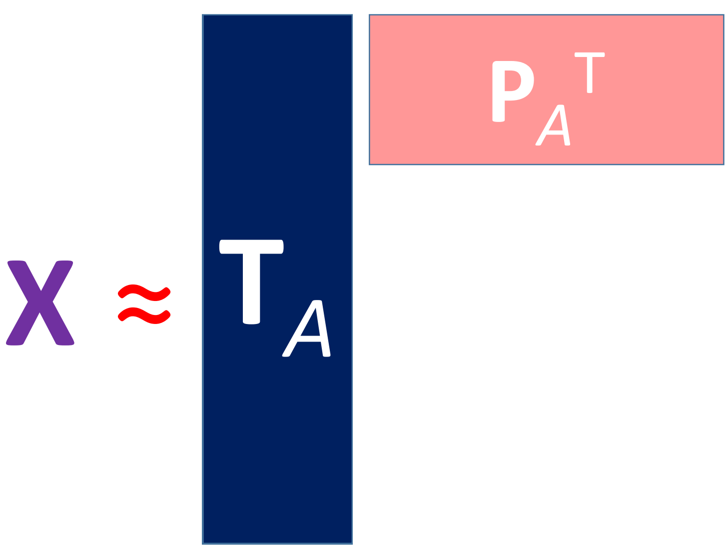
Aggregate real panel data



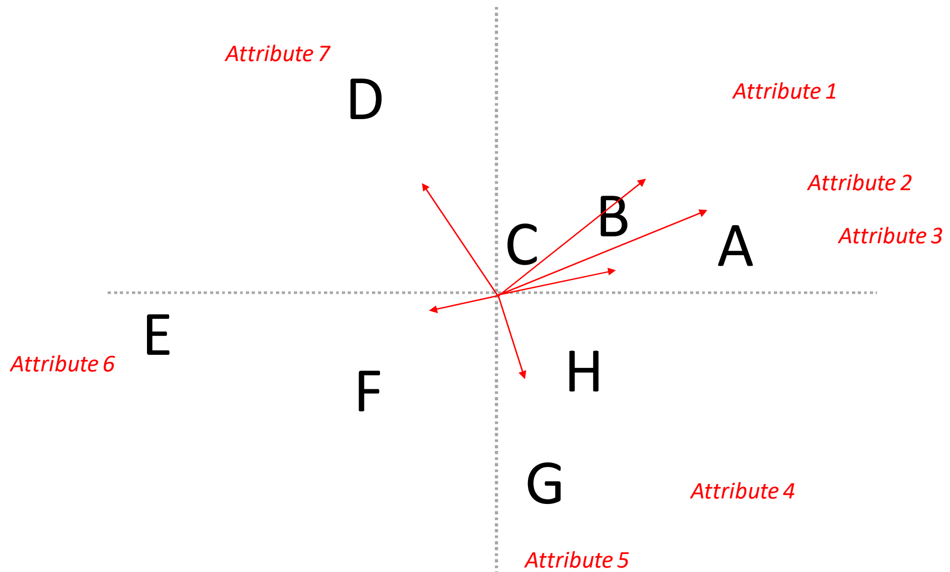
Principal Component Analysis



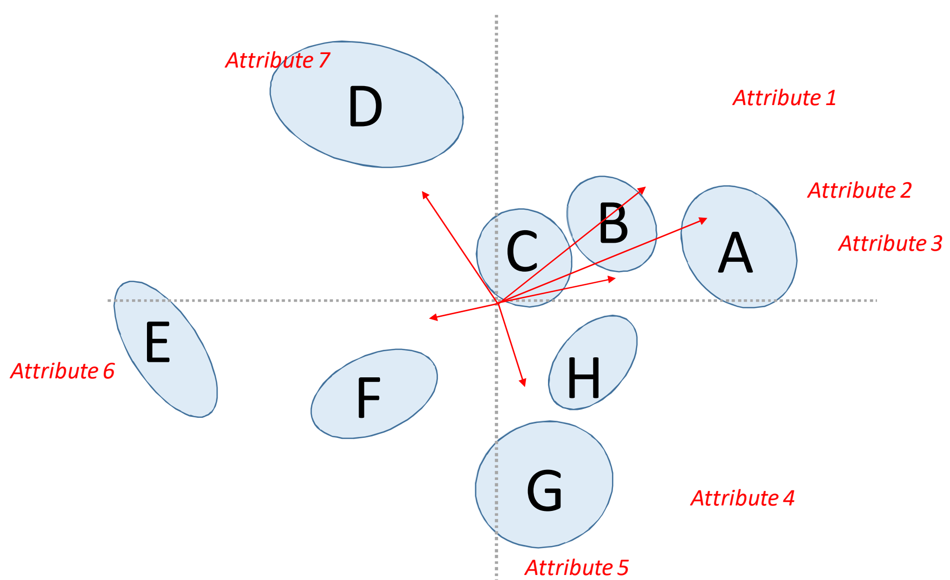
Dimension Reduction

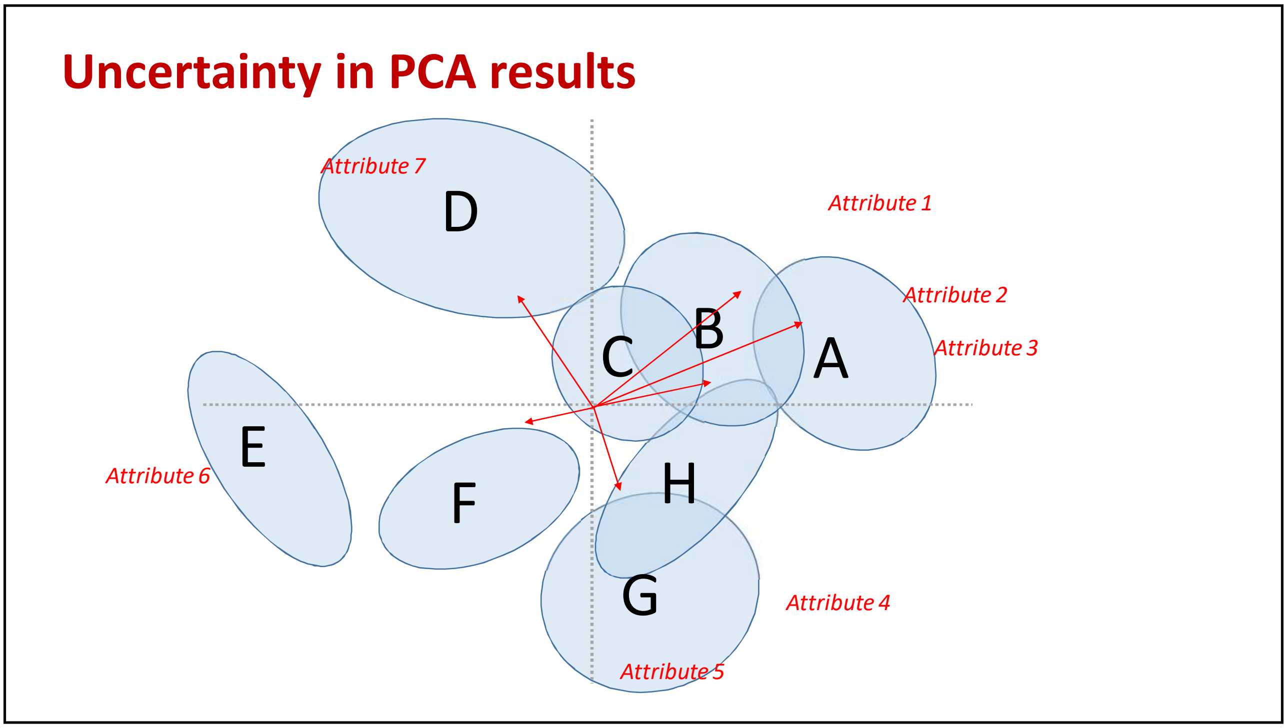


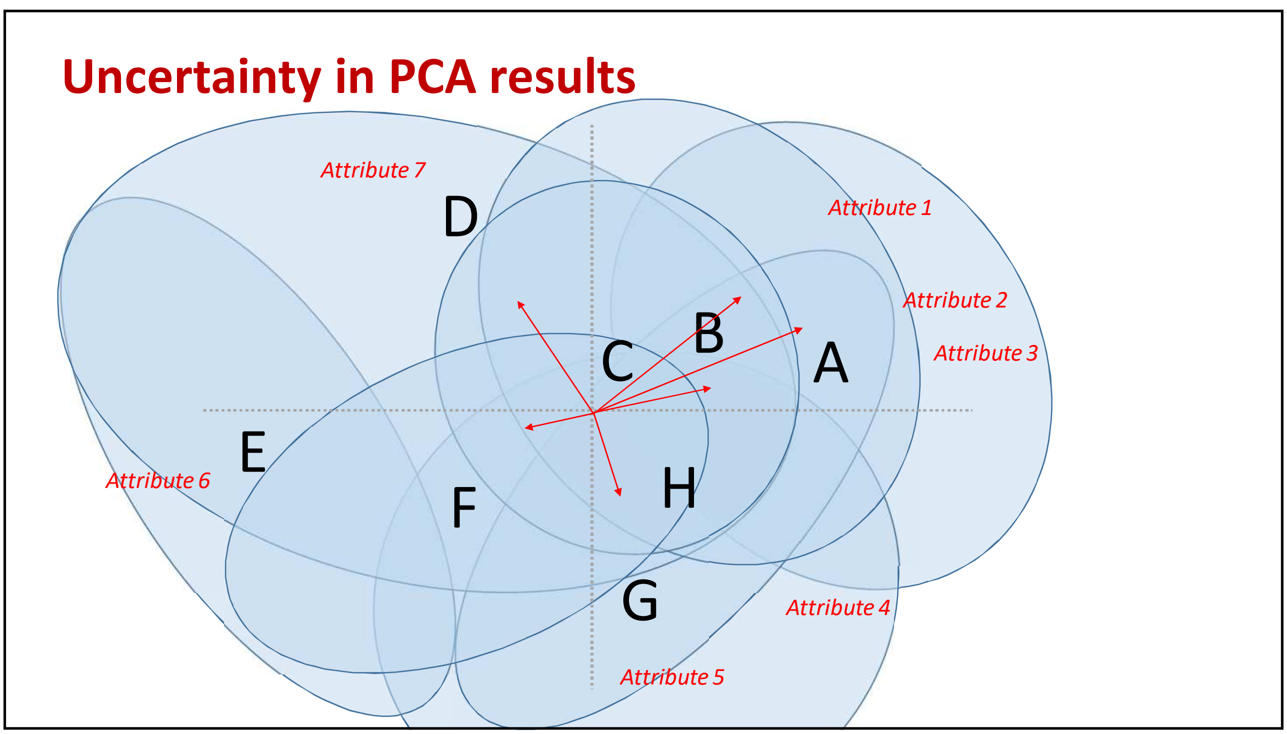
PCA results



Uncertainty in PCA results




Uncertainty in PCA results
Attribute 7
D
Attribute 1
B
Attribute 2
C
A
Attribute 3
E
Attribute 6
F
H
G
Attribute 4
Attribute 5

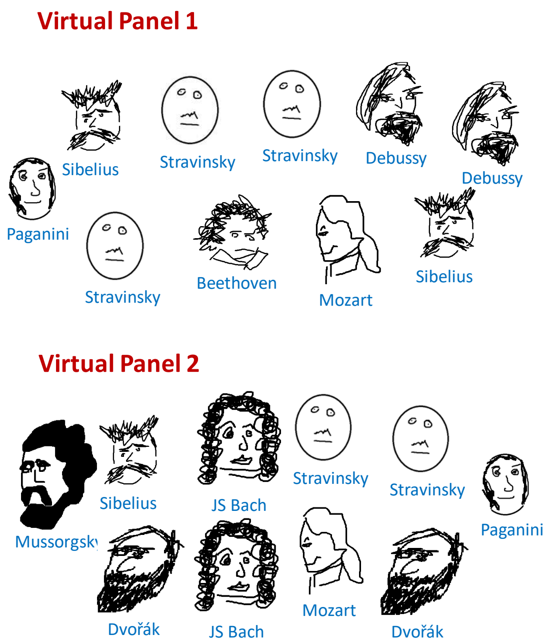

Uncertainty in PCA results
Attribute 7
D
Attribute 1
Attribute 2
B
C
A
Attribute 3
E
Attribute 6
F
H
G
Attribute 4
Attribute 5

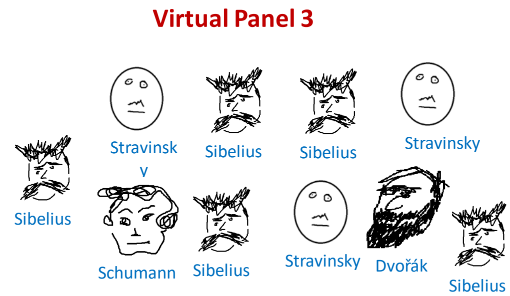
Truncated
Total Bootstrap Procedure

(Cadoret & Husson, 2013)

Now we use the bootstrap procedure to compose many virtual panels, each the same size as the original panel.

We sample the real assessors with replacement, so some assessors might be chosen for a virtual panel multiple times, whereas other assessors might not be chosen at all for that virtual panel.

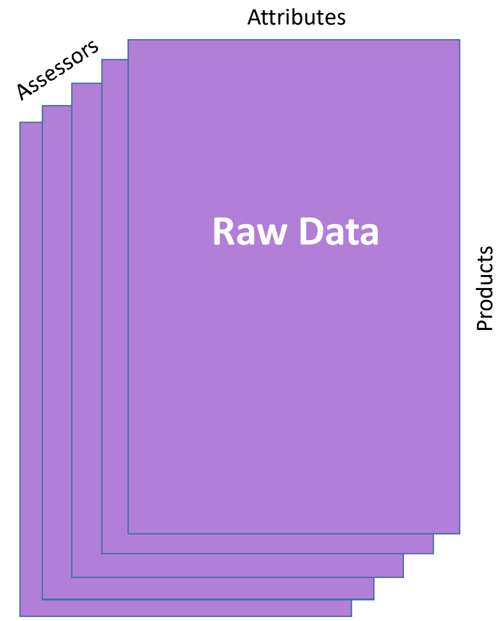




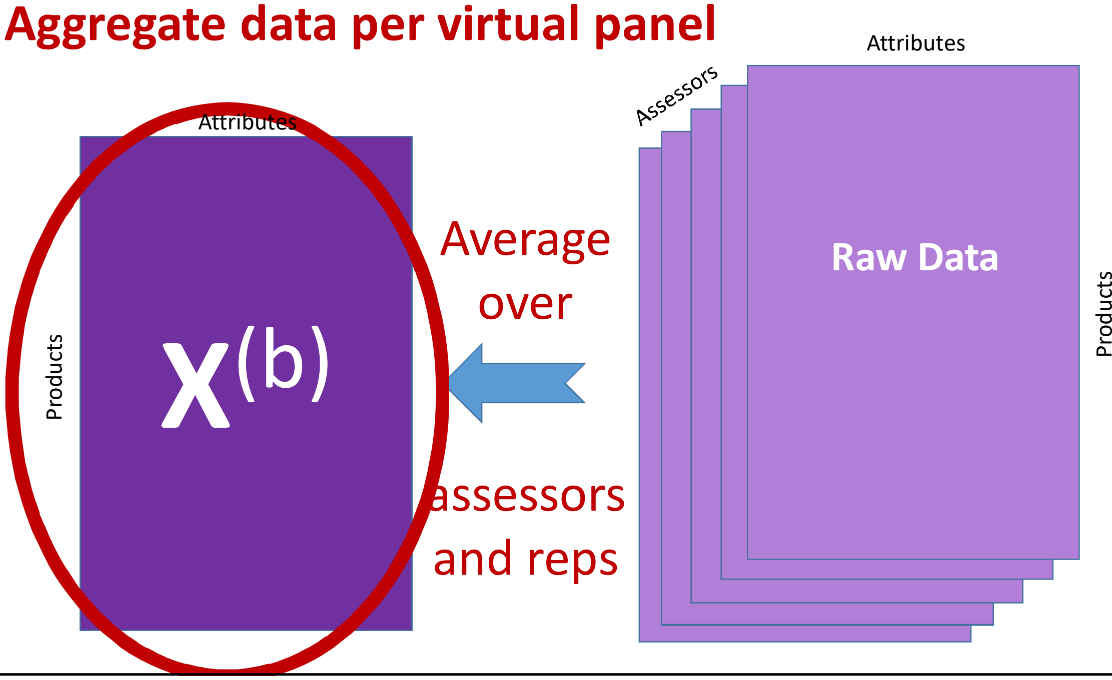
…and so on to create B virtual panels. (B is large.)

The results of the virtual panels are analyzed identically to the real panel.

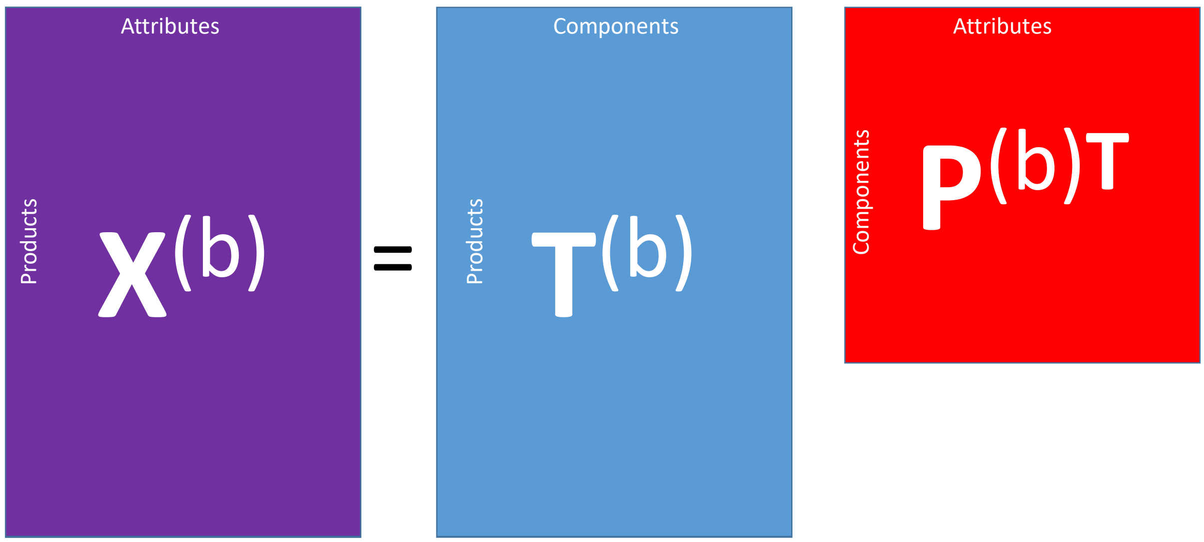
Data from a virtual panel



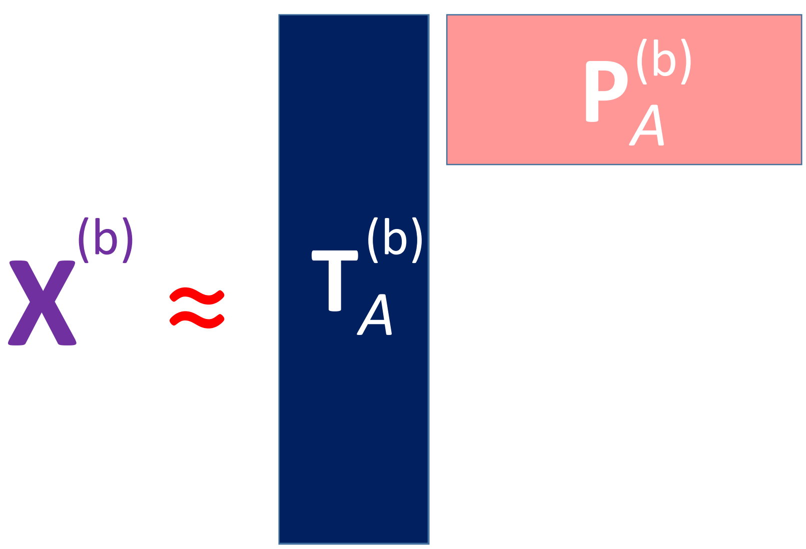
Aggregate data per virtual panel



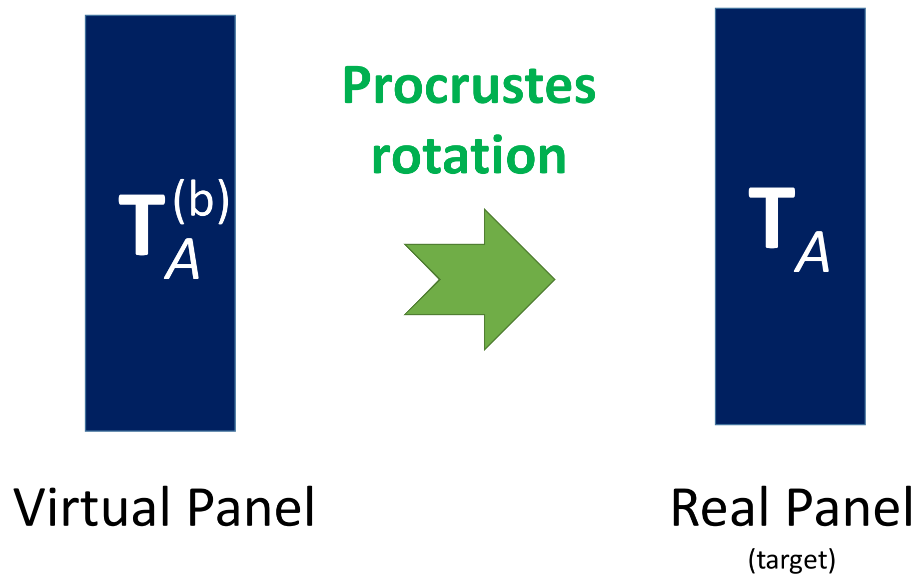
PCA of column-centered matrix



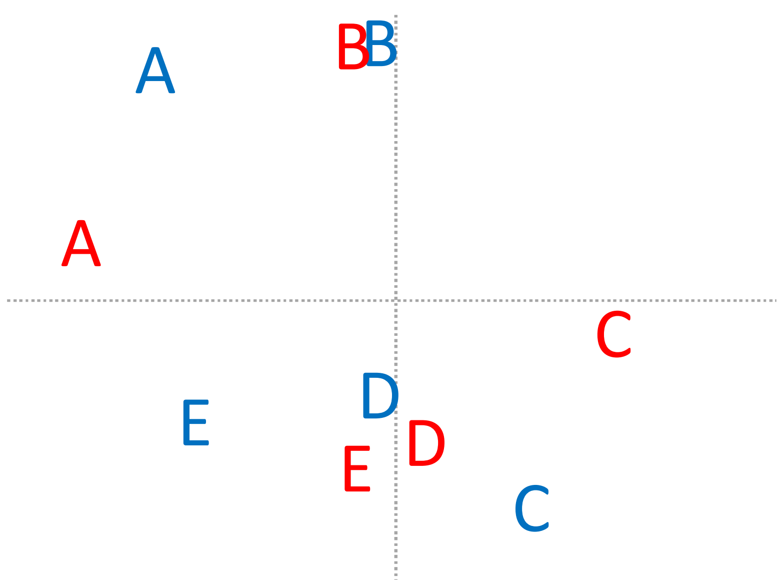
Dimension Reduction



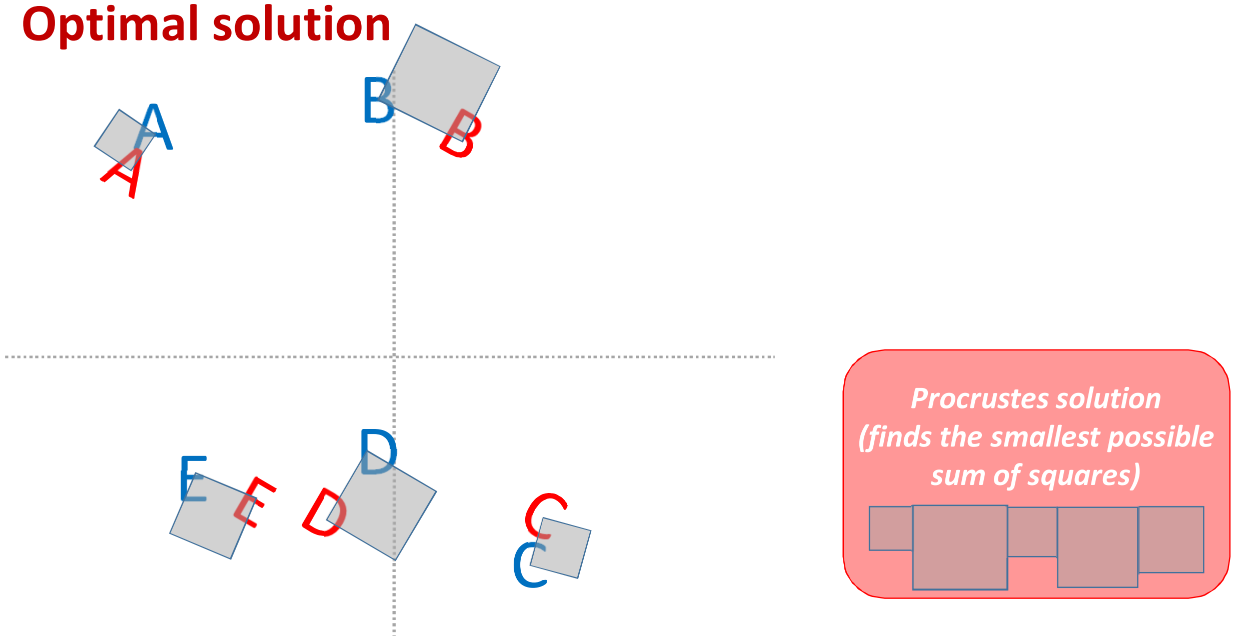
Superimpose on real product configuration

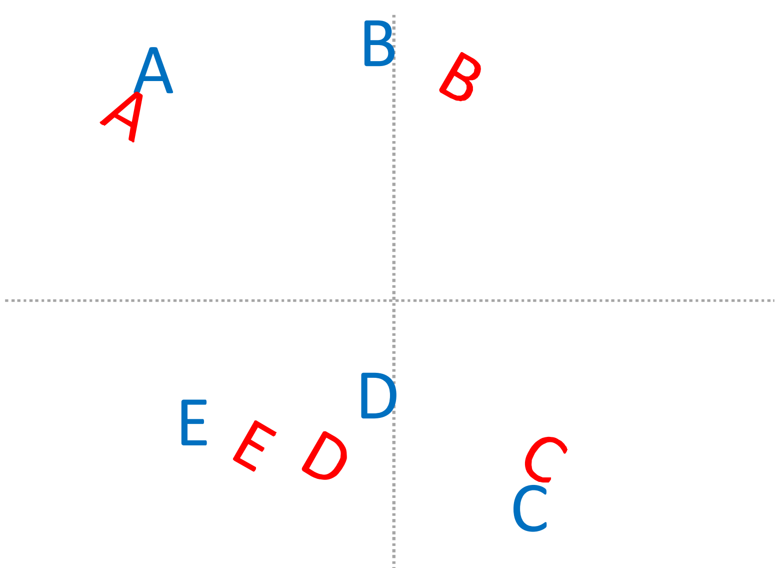


Optimal solution



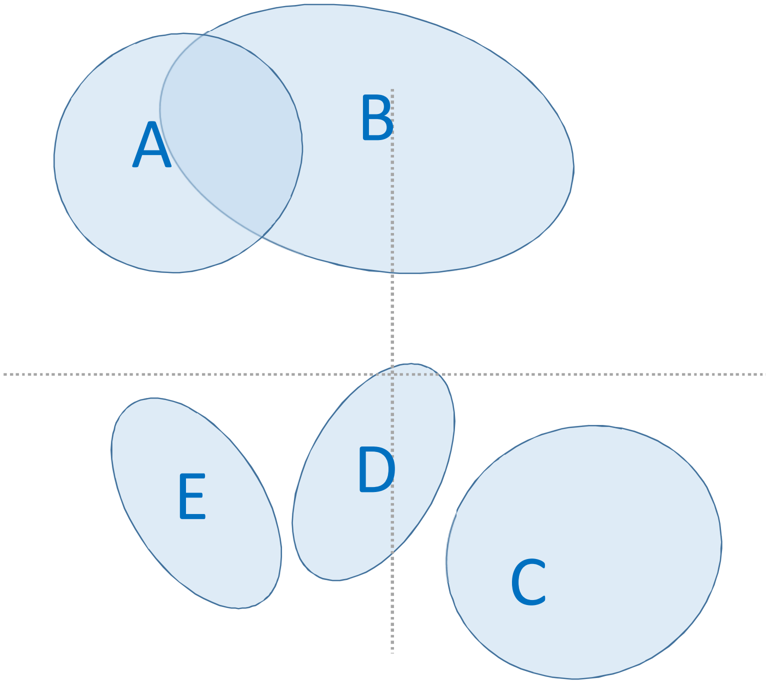
Optimal solution





This is one of many virtual panels.

We do the same for many virtual panels.



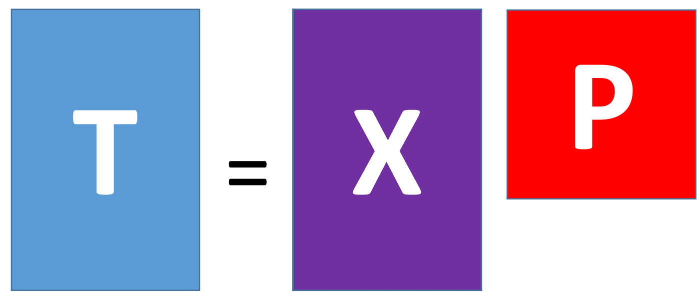
Then we use these results to get **TTB-derived confidence ellipsoids**.

New developments!

Paired Comparisons after PCA

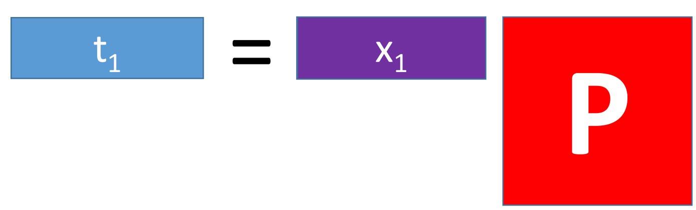
Principal Component Analysis

$\mathbf{T} = \mathbf{X}\mathbf{P}$

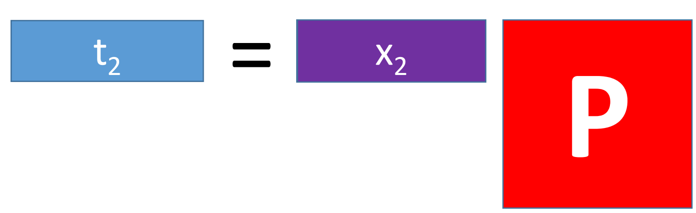


Multiplying data by loadings gives scores

$\mathbf{t}_1^T = \mathbf{x}_1^T \mathbf{P}_A$



$\mathbf{t}_2^T = \mathbf{x}_2^T \mathbf{P}_A$



Differences between two scores

$$(t_1 - t_2) = (x_1 - x_2)$$

P

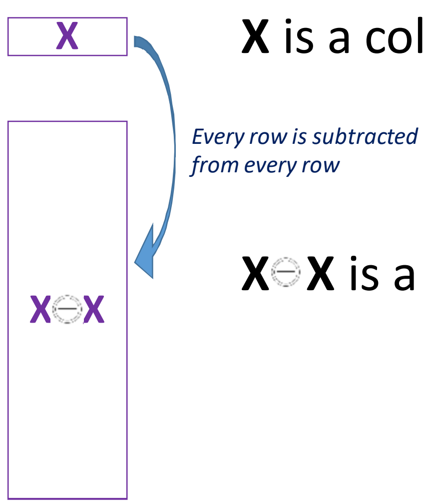
But this does not demonstrate that paired comparisons are optimally investigated in these components.

A demonstration that the space is identical is given in this paper, currently under review:

Castura, J.C., Varela, P., & Næs, T. (n.d.). Investigating paired comparisons after principal component analysis. *Food Quality and Preference, under review*.

Some highlights follow.

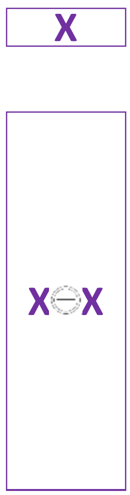
"Crossdiff-unfolding"



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

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

“Crossdiff-unfolding”

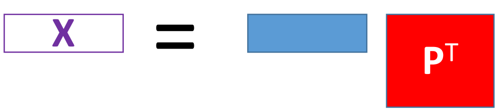


The covariance matrix of **X** and the covariance matrix of **X**⊖**X** are identical except for a multiplier.

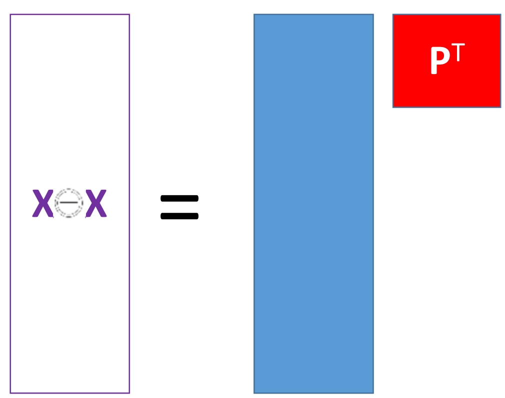
Next, we consider PCA of **X** and PCA of **X**⊖**X**.

Key relationships

PCA of X

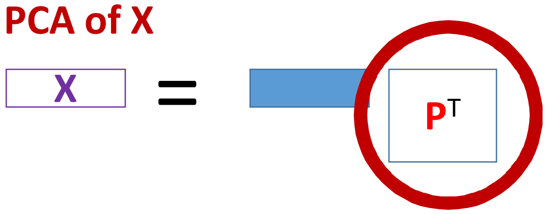


PCA of X⊖X



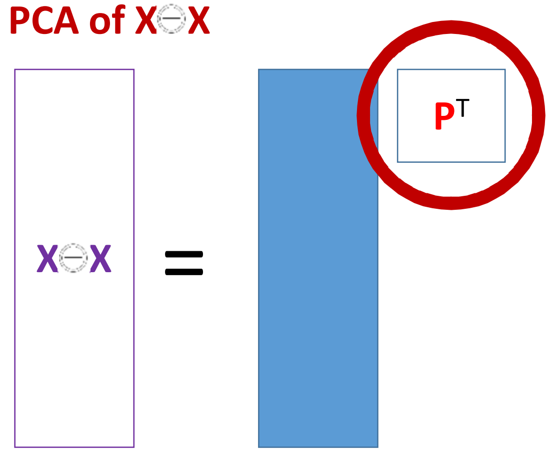
Key relationships

PCA of X



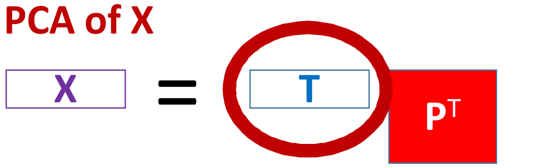
Key result #1:
Loading matrices obtained from these two PCA solutions are identical.

PCA of X⊖X



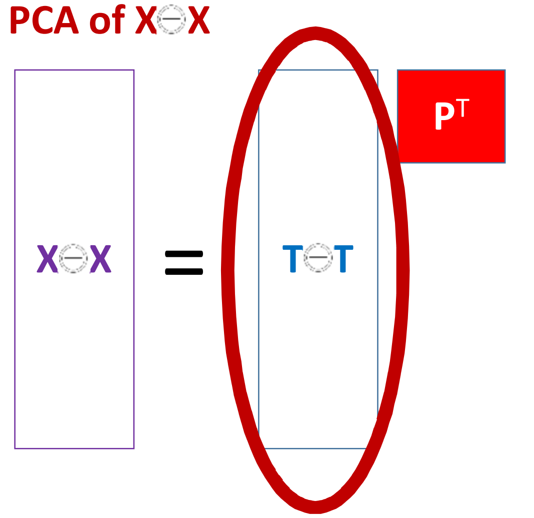
Key relationships

PCA of X



Key result #2:
If we crossdiff-unfold scores from PCA of X, we get scores from PCA of X⊖X.

PCA of X⊖X



Paired comparisons

This shows 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 get results for 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.

Principal Component Analysis

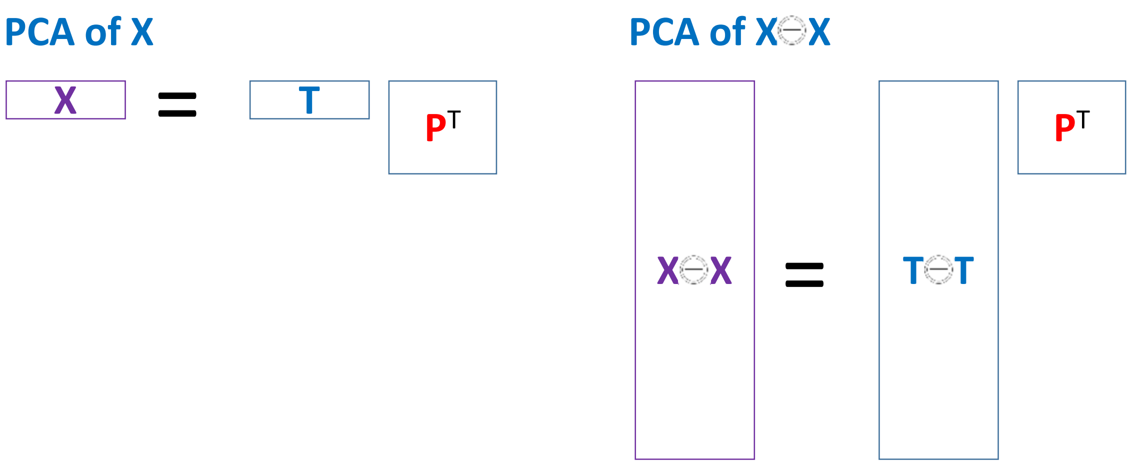
Uncertainty in

Paired Comparisons after PCA

The same Procrustes rotation matrix that superimposes $\mathbf{T}^{(b)}$ on $\mathbf{T}$ also superimposes $\mathbf{T}^{(b)} \ominus \mathbf{T}^{(b)}$ on $\mathbf{T} \ominus \mathbf{T}$. This demonstration is given in…

Castura, J.C., Varela, P., & Næs, T. (n.d.). Investigating paired comparisons after principal component analysis. *Food Quality and Preference, under review*.

...together with results presented earlier...



...allows us to investigate paired comparisons easily.

We can obtain clouds of TTB-derived scores for the real-panel scores based on

$$\mathbf{X} = \mathbf{T}\mathbf{P}^{T}$$

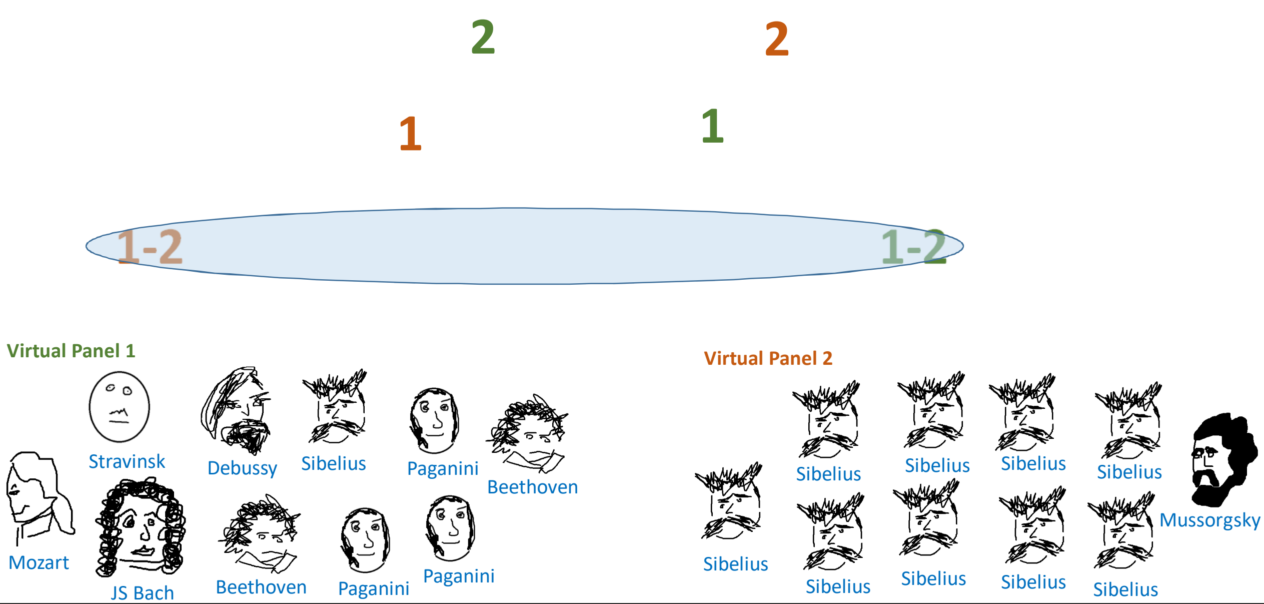
then obtain the TTB-derived paired difference scores.

Confidence ellipses for paired comparisons

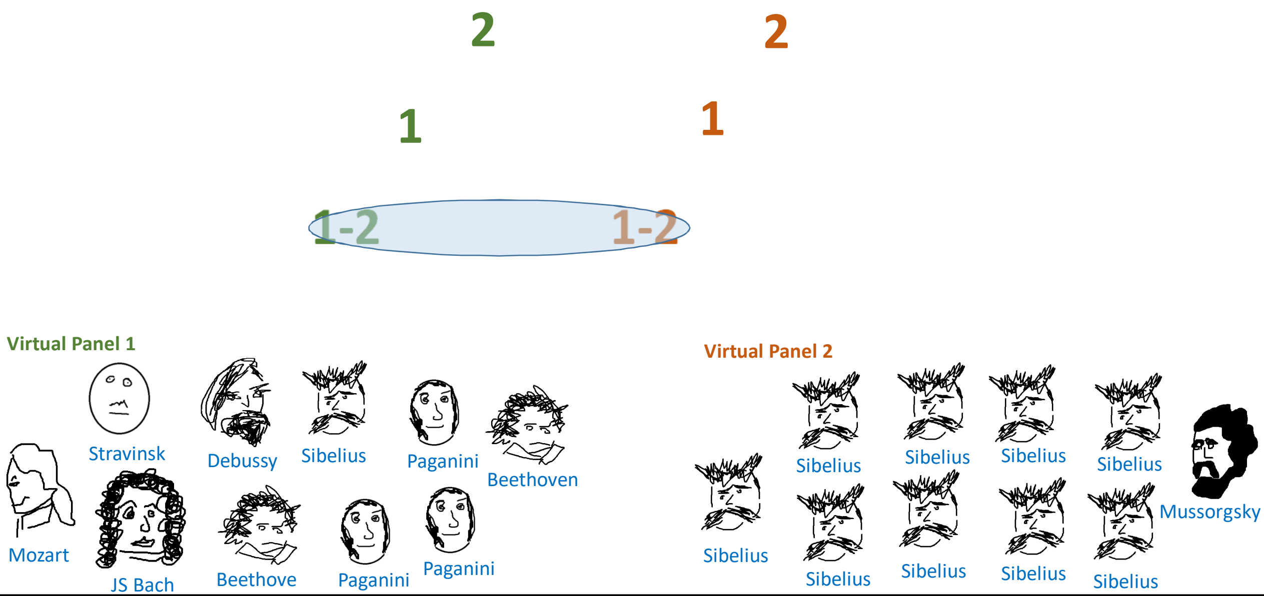
2 2

1 1

Confidence ellipses for paired comparisons



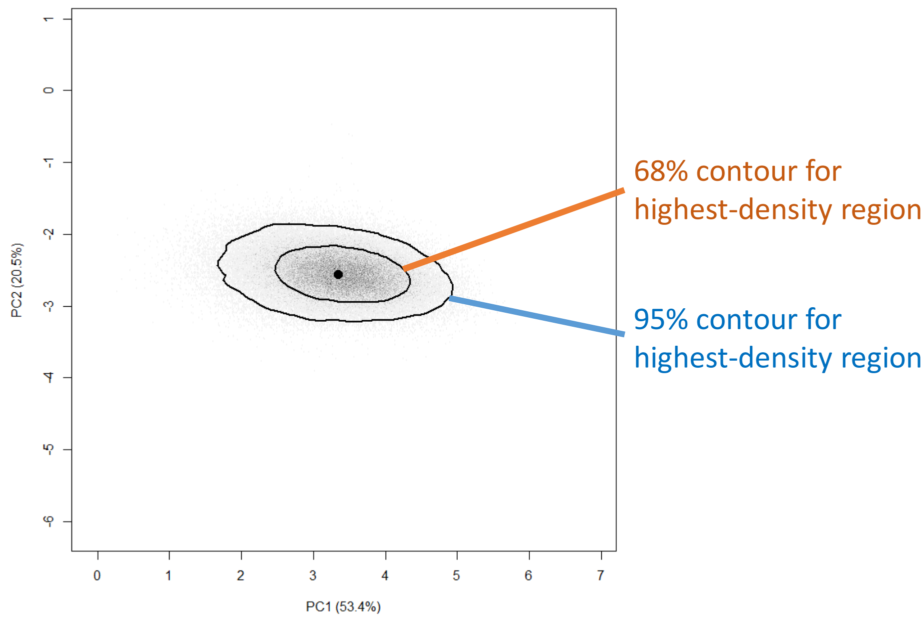
Confidence ellipses for paired comparisons



This indicates that we need to **account for mutual dependencies in the TTB-derived results** when investigating paired comparisons.

Kernel-based density estimation

for visualizing the uncertainty of a paired difference



Is it reasonable to obtain confidence ellipsoids for these TTB-derived clouds of points?

An ellipsoidal shape assumes that the underlying distribution is multinormal.

But some of our clouds have excess kurtosis and skewness.

For some time, many people visualize confidence ellipses for objects after PCA using this and other methods.

So it is very relevant to know: is a confidence ellipsoid valid if the underlying distribution is not really multinormal?

This topic is investigated in another paper under review with FQAP.

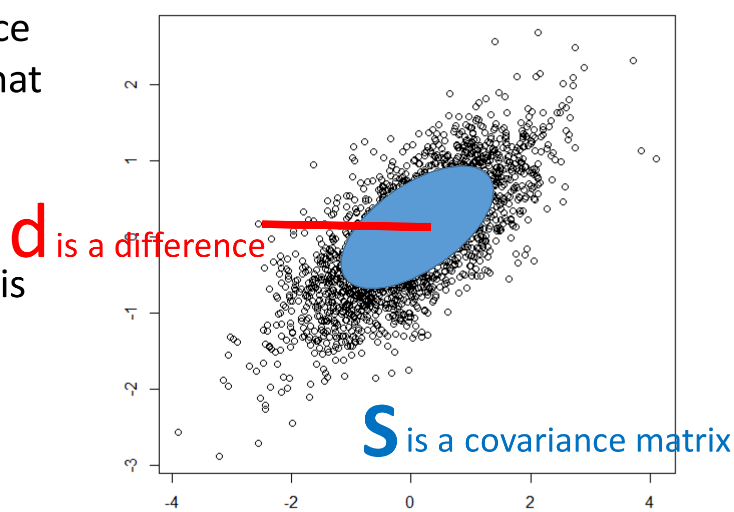
Castura, J.C., Varela, P., & Næs, T. (n.d.) Evaluation of complementary numerical and visual approaches for investigating pairwise comparisons after principal component analysis. *Food Quality and Preference*, under review.

Mahalanobis distance

The Mahalanobis distance is a statistical distance that scales the distance according to variability.

The <u>squared</u> Mahalanobis distance is

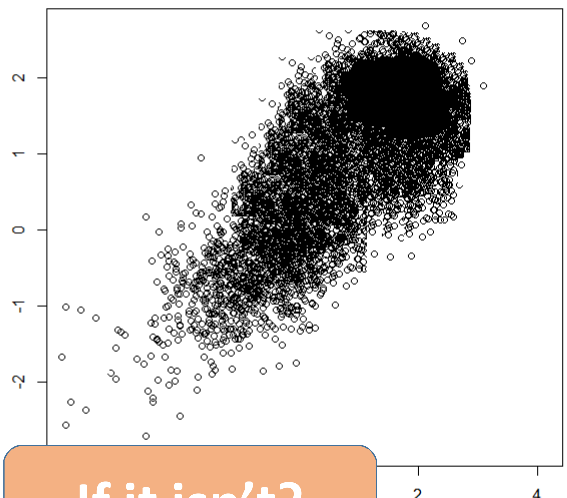
$$D^2 = d^T S^{-1} d$$



Multinormally distributed cloud of points

$$\chi^2 \sim d^T S^{-1} d$$

Infinite points would be χ^2 distributed with *A* degrees of freedom **if the data generating process were truly multinormal in *A* dimensions**.

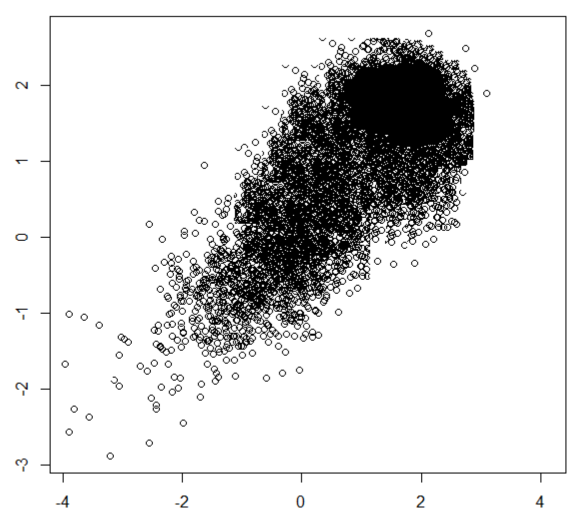


If it isn't?

What if the points are not distributed multinormally?

We want a consistent approach. Since we cannot guarantee that the distribution will be multinormal, we rely instead on the empirical null distribution

$$Q \sim d^T S^{-1} d$$

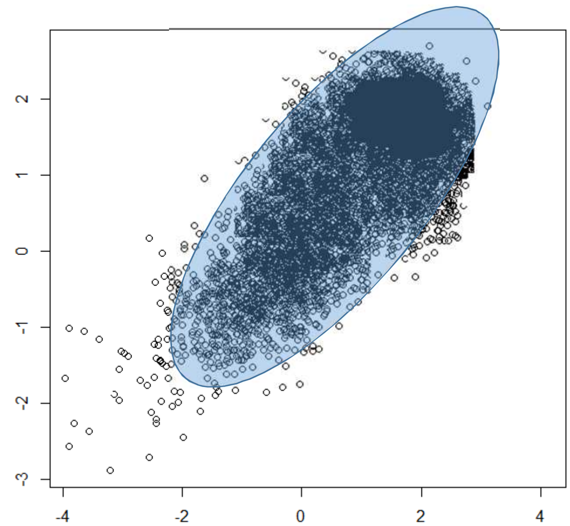


What if the points are not distributed multinormally?

Q_c is the 95th quantile of Q. So 95% of points satisfy

$$Q_c \geq \mathbf{d}^T \mathbf{S}^{-1} \mathbf{d}$$

A point that is outside the ellipsoid is “unusual” and will be flagged for review.



Screening using a P value

Squared Mahalanobis distance between products (based on real panel)

$$P = \Pr\left(\mathbf{d}^T \mathbf{S}^{-1} \mathbf{d} > Q \mid H_0\right)$$

covariance matrix

squared Mahalanobis distances of null distribution (based on virtual panels)

95% confidence ellipsoid

What are we "confident" about?

And why are we "95%" confident?

Results from our simulation studies indicate that this statements is *approximately* true…

We are 95% confident that the ellipsoid contains the true parameter value because it is constructed by a procedure such that under repetition 95% of such ellipsoids contain the true parameter value.

Confidence ellipsoids vs density regions

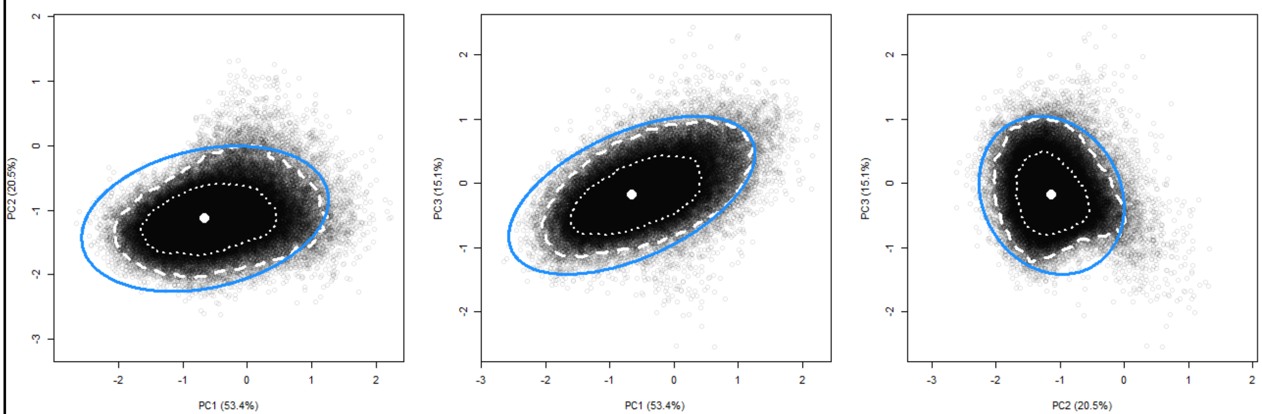
Earlier we showed how to obtain regions containing 95% of the kernel-estimated densities based on the TTB-derived clouds of points. These density regions do not assume a statistical distribution.

How do these density regions compare with the confidence ellipsoids?

Application to real data sets

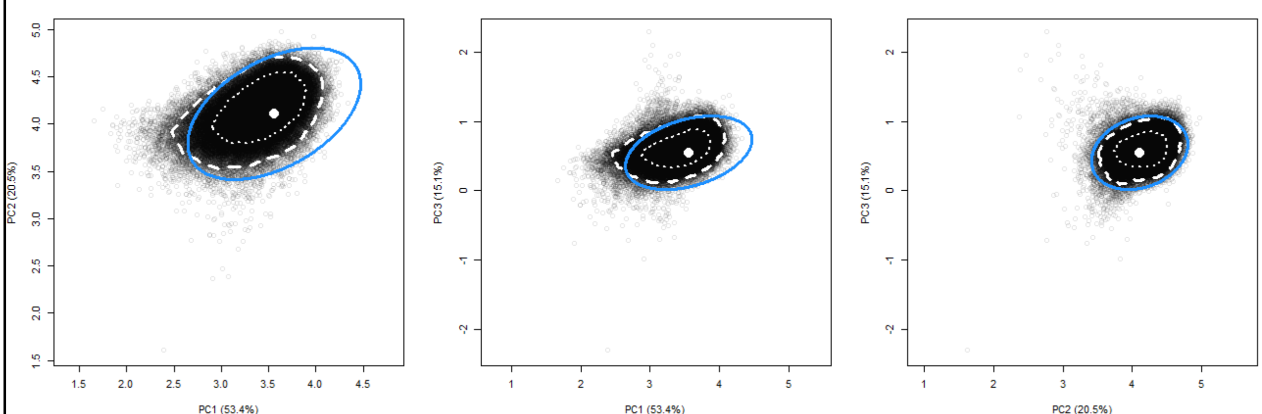
Beverages

Almond (1)



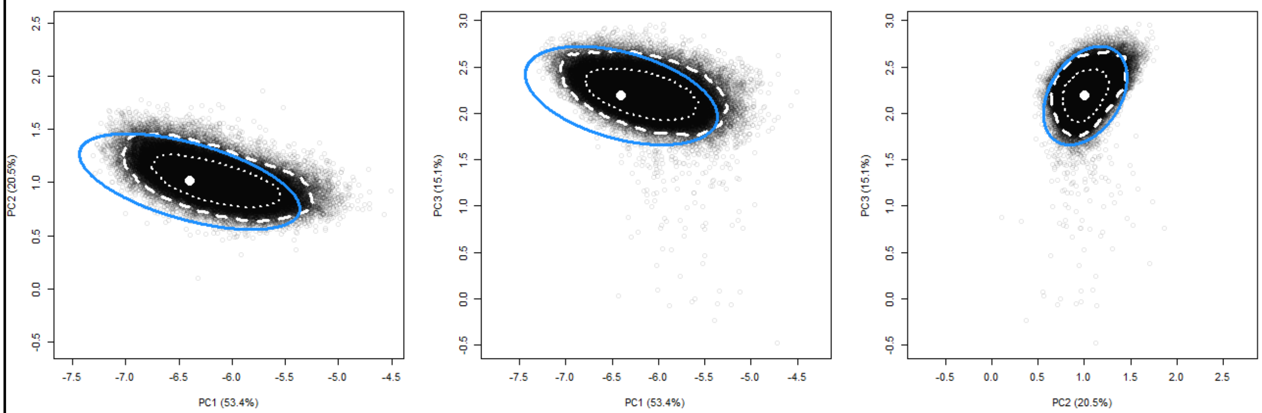
Beverages

Coconut (2)



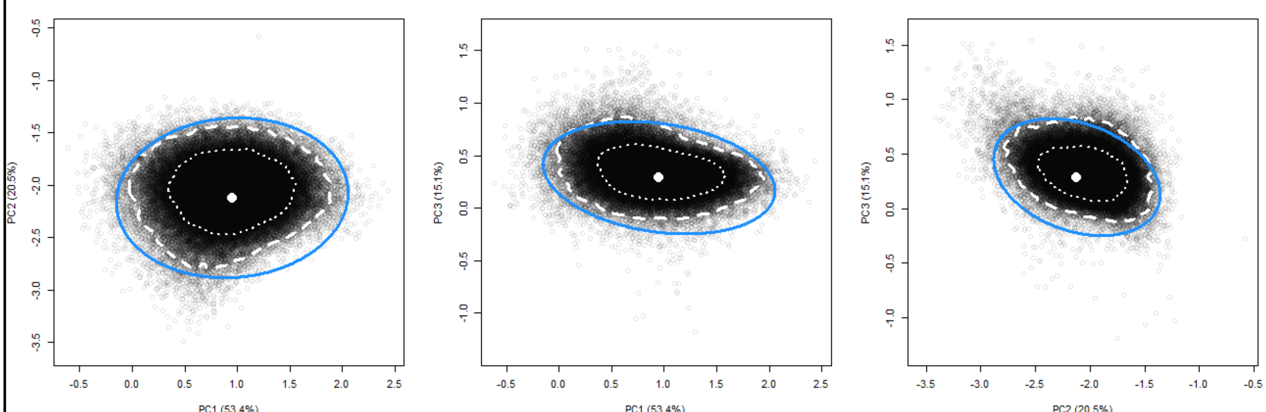
Beverages

Cow milk (3)

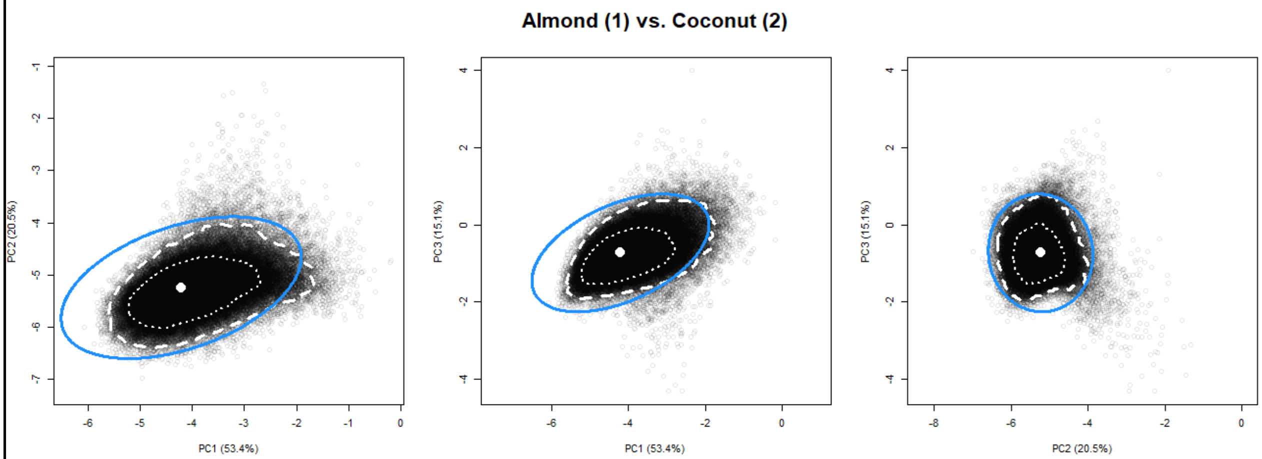


Beverages

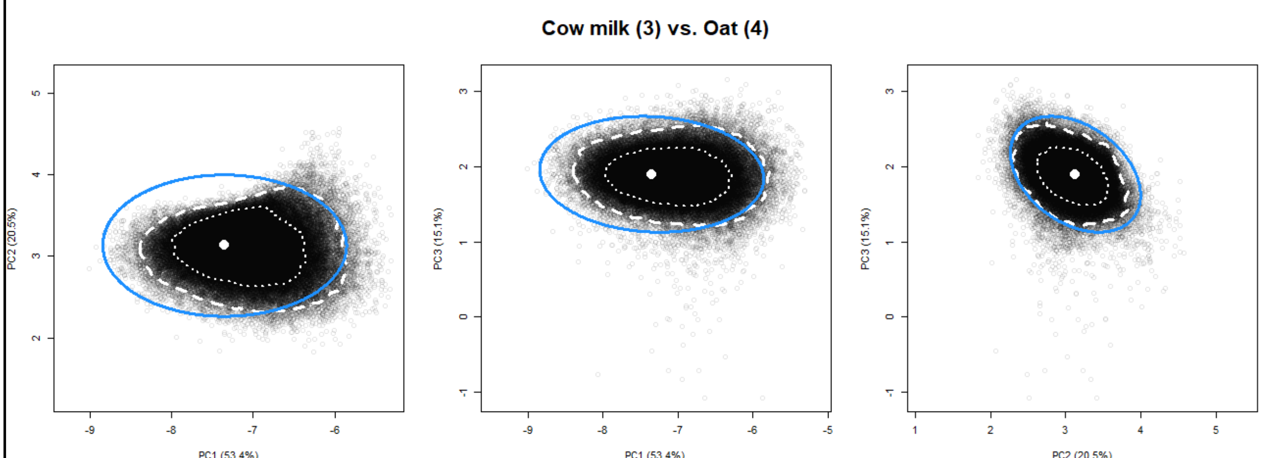
Oat (4)



Pairs of Beverages

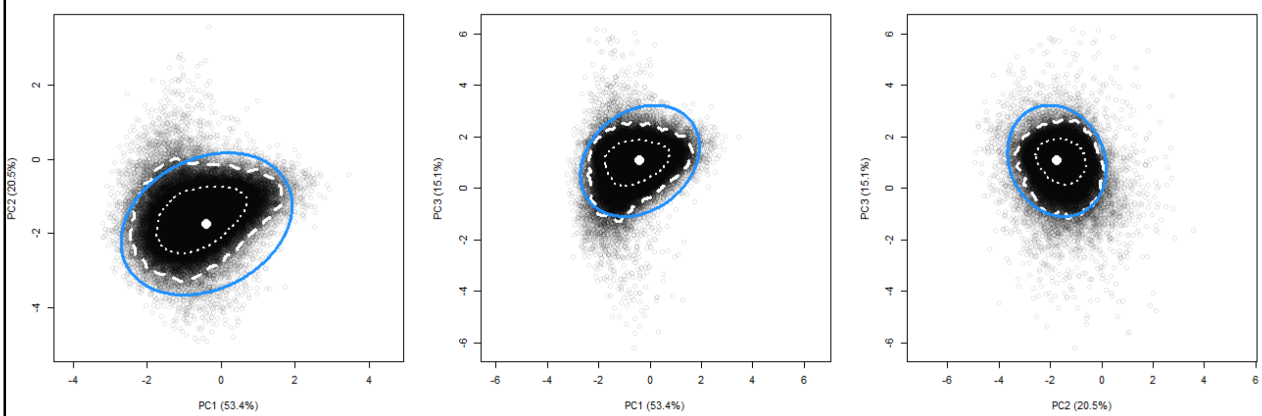


Pairs of Beverages



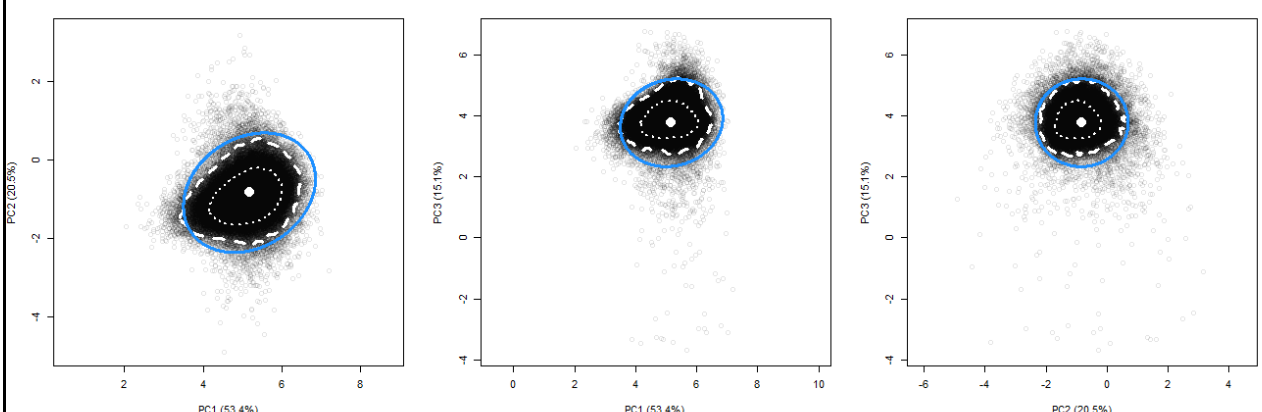
Pairs of Beverages

Peas (5) vs. Rice (6)



Pairs of Beverages

Rice (6) vs. Soya (7)



Pairs of Beverages – ellipsoid volumes

The volume of 95% confidence ellipsoid for all beverages (main diagonal, underlined) and their paired comparisons (lower triangle, plain text) are shown. [(1) Almond; (2) Coconut; (3) Cow Milk; (4) Oat; (5) Peas; (6) Rice; (7) Soya.]

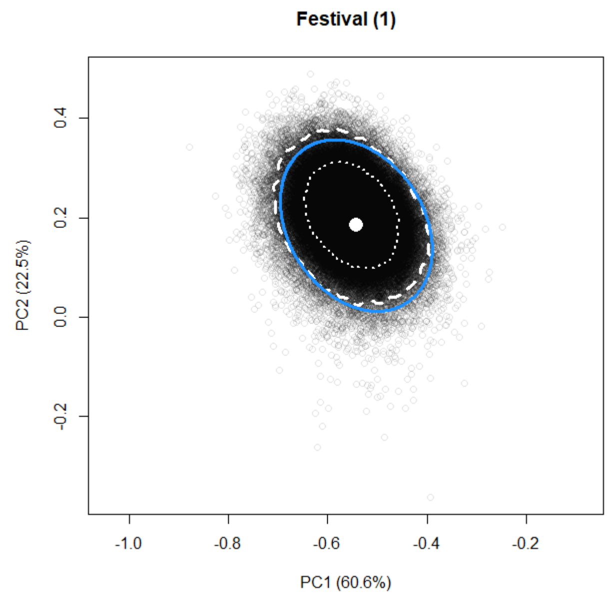
	1	2	3	4	5	6	7
1	8.6						
2	15.0	1.2					
3	17.5	3.3	0.8				
4	19.4	3.2	3.9	1.8			
5	36.6	10.2	10.5	16.9	6.7		
6	18.2	15.2	10.1	11.2	36.6	6.1	
7	19.6	4.4	3.9	5.1	5.6	14.9	1.5

Pairs of Beverages – P values

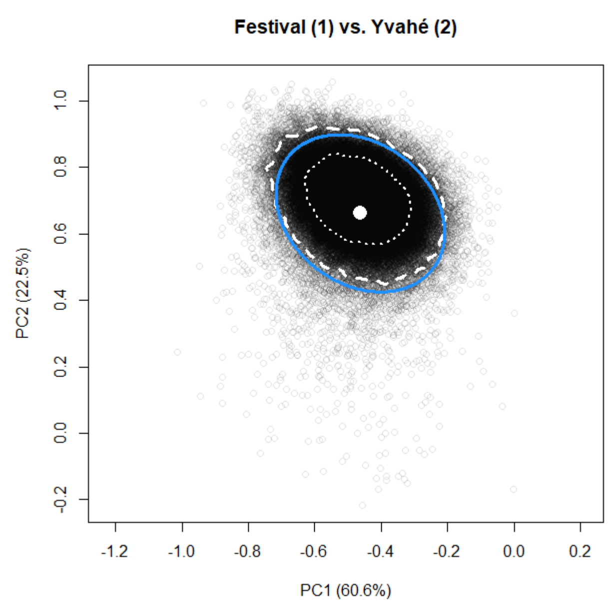
P values are shown for the beverages (main diagonal) and their paired comparisons (lower triangle). Beverages that are discriminated from the origin and beverage pairs that are discriminated with 95% confidence are shown in bold. [(1) Almond; (2) Coconut; (3) Cow Milk; (4) Oat; (5) Peas; (6) Rice; (7) Soya.]

	1	2	3	4	5	6	7
1	**0.036**						
2	**<0.001**	**<0.001**					
3	**<0.001**	**<0.001**	**<0.001**				
4	0.050	**<0.001**	**<0.001**	**<0.001**			
5	**0.010**	**<0.001**	**<0.001**	0.201	**<0.001**		
6	**0.003**	**<0.001**	**<0.001**	**0.007**	0.055	**0.001**	
7	**0.001**	**<0.001**	**<0.001**	**<0.001**	**<0.001**	**<0.001**	**<0.001**

Strawberry cultivars



Pairs of strawberry cultivars



Pairs of Strawberry Cultivars – ellipsoid volumes

The 95% confidence ellipse volumes are shown for all strawberry cultivars (main diagonal, underlined) and their paired comparisons (lower triangle, plain text). [Strawberry cultivars: (1) Festival, (2) Yvahé, (3) Yurí, (4) Guenoa, (5) L20.1, and (6) K31.5.]

	1	2	3	4	5	6
1	<u>0.08</u>					
2	0.18	<u>0.09</u>				
3	0.31	0.34	<u>0.19</u>			
4	0.17	0.20	0.27	<u>0.08</u>		
5	0.15	0.16	0.34	0.23	<u>0.08</u>	
6	0.39	0.34	0.60	0.31	0.28	<u>0.20</u>

Pairs of Strawberry Cultivars – P values

P values are shown for the strawberry cultivars (main diagonal) and their paired comparisons (lower triangle). Strawberry cultivars that are discriminated from the origin and cultivar pairs that are discriminated with 95% confidence are shown in bold. [(1) Festival, (2) Yvahé, (3) Yurí, (4) Guenoa, (5) L20.1, and (6) K31.5.]

	1	2	3	4	5	6
1	**<0.001**					
2	**<0.001**	**<0.001**				
3	**<0.001**	**0.005**	**0.851**			
4	**<0.001**	**<0.001**	**0.001**	**<0.001**		
5	**<0.001**	**<0.001**	**<0.001**	**0.036**	**<0.001**	
6	0.132	**0.002**	0.241	**<0.001**	**<0.001**	**<0.001**

1. Researcher designs experiment and collects data.

2. Data analysis.

Automated data analysis.
Screening for unusual results.
Visualizations for review.

3. Interpretation of results.

4. Recommendations and decisions.

Selected References

Cadoret, M., & Husson, F. (2013). Construction and evaluation of confidence ellipses applied at sensory data. *Food Quality and Preference*, *28*, 106-115.

Castura, J.C., Varela, P., & Næs, T. (n.d.). Investigating paired comparisons after principal component analysis. *Food Quality and Preference*, under review.

Castura, J.C., Varela, P., & Næs, T. (n.d.) Evaluation of complementary numerical and visual approaches for investigating pairwise comparisons after principal component analysis. *Food Quality and Preference*, under review.

Thank you for your attention.

John Castura

Paula Varela

Tormod Næs

Compusense

Nofima

For further information, please contact **jcastura@compusense.com**