Investigating paired differences for data sets with special structures after PCA

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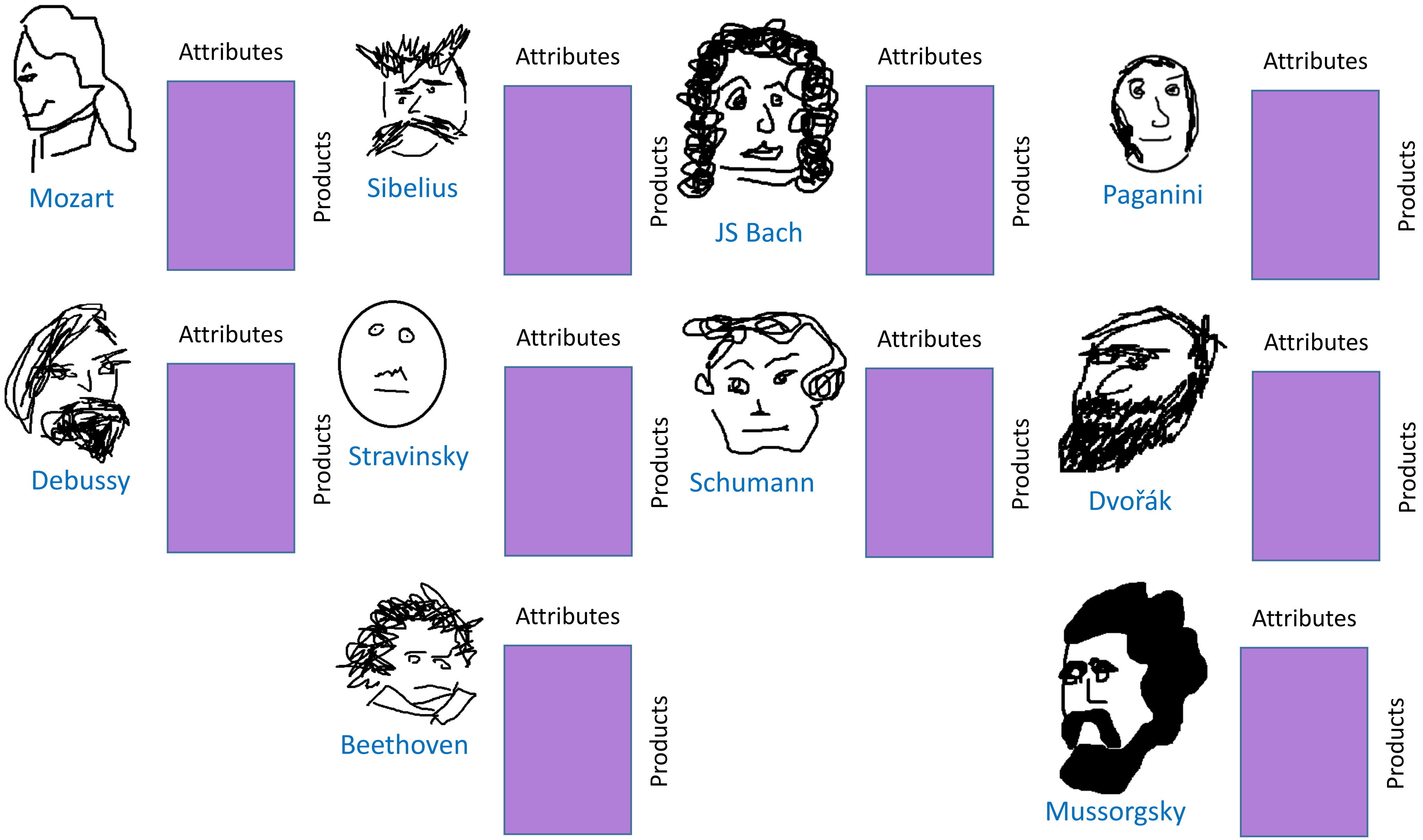
A typical application of **principal component analysis** in sensory evaluation

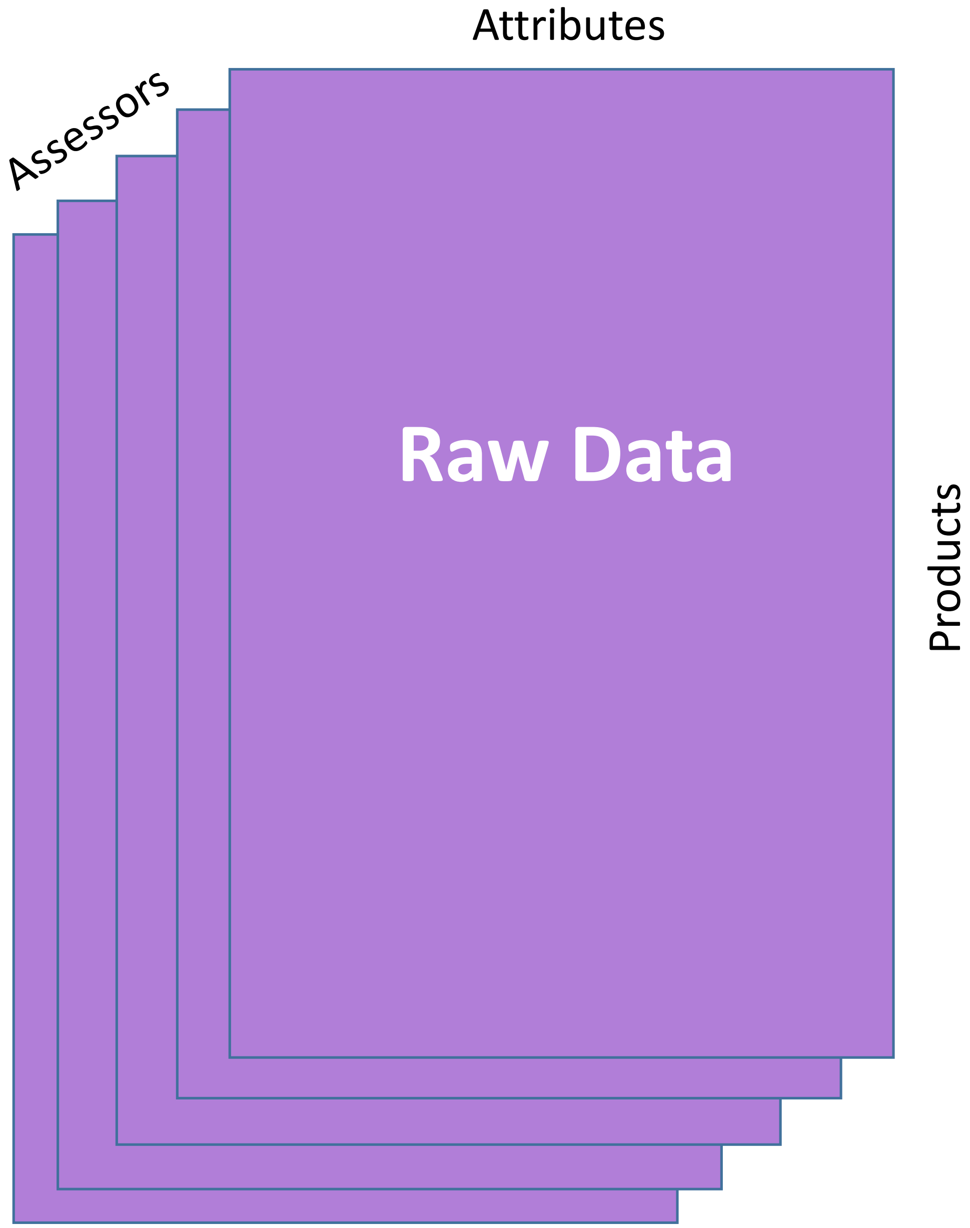
Panel of Trained Sensory Assessors

Illustration credit: J.C. Castura

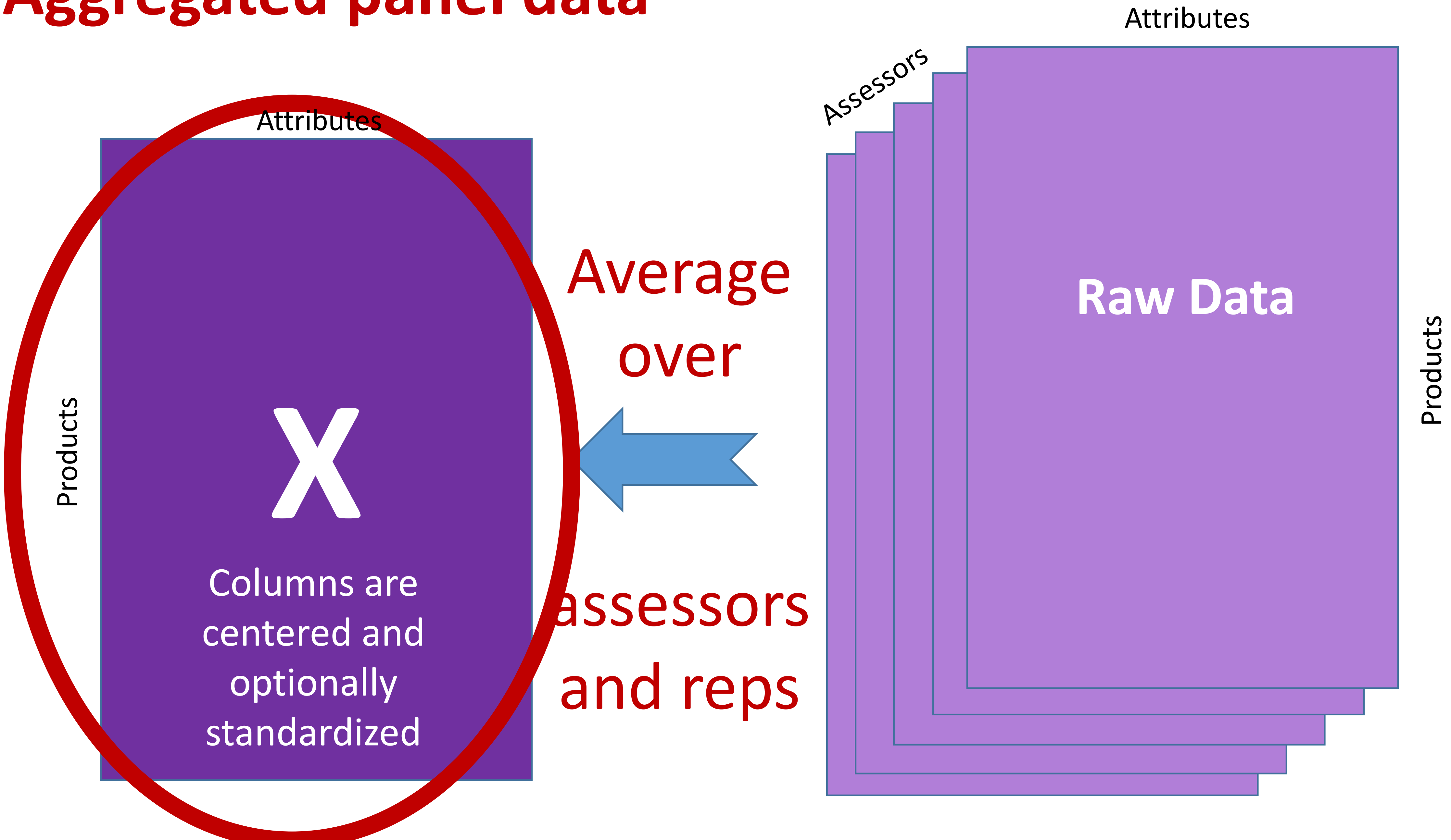
Data from a trained sensory panel



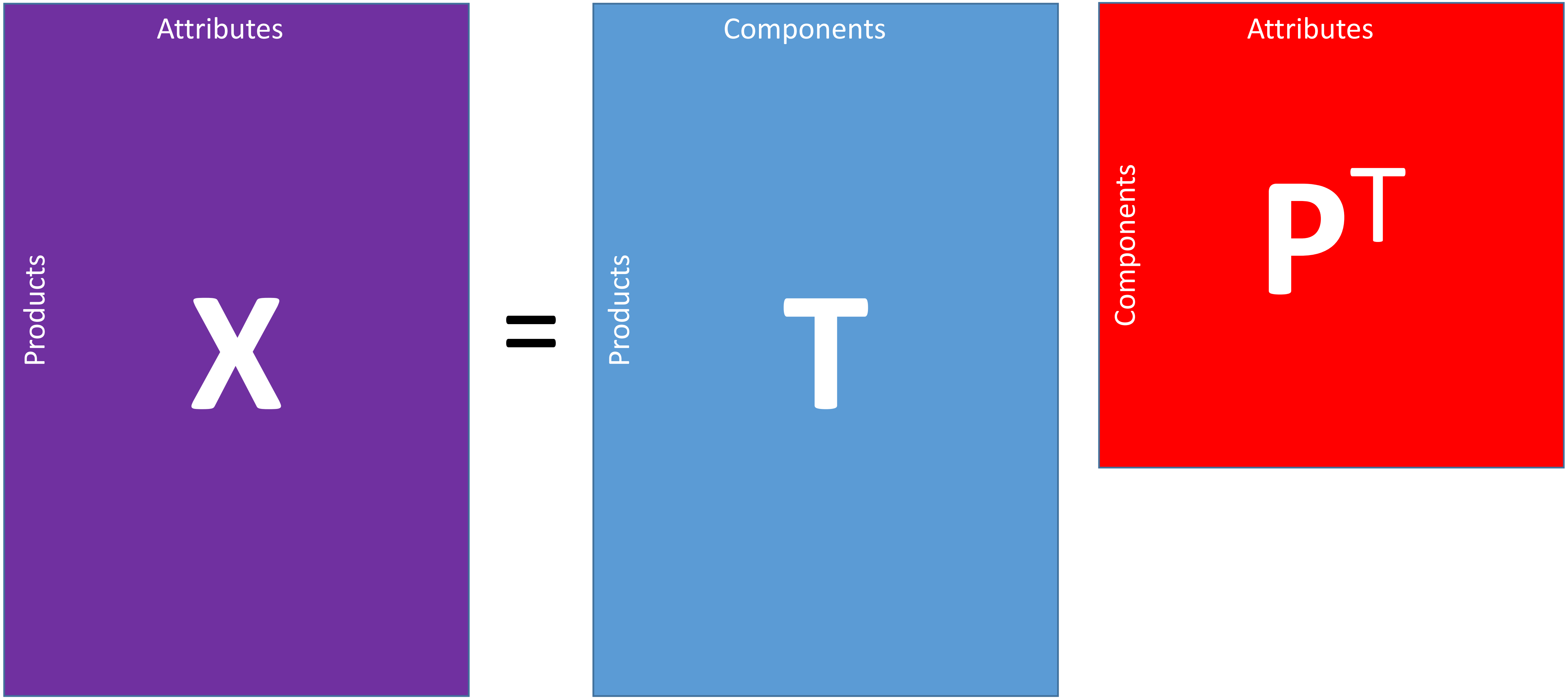
Panel data



Aggregated panel data

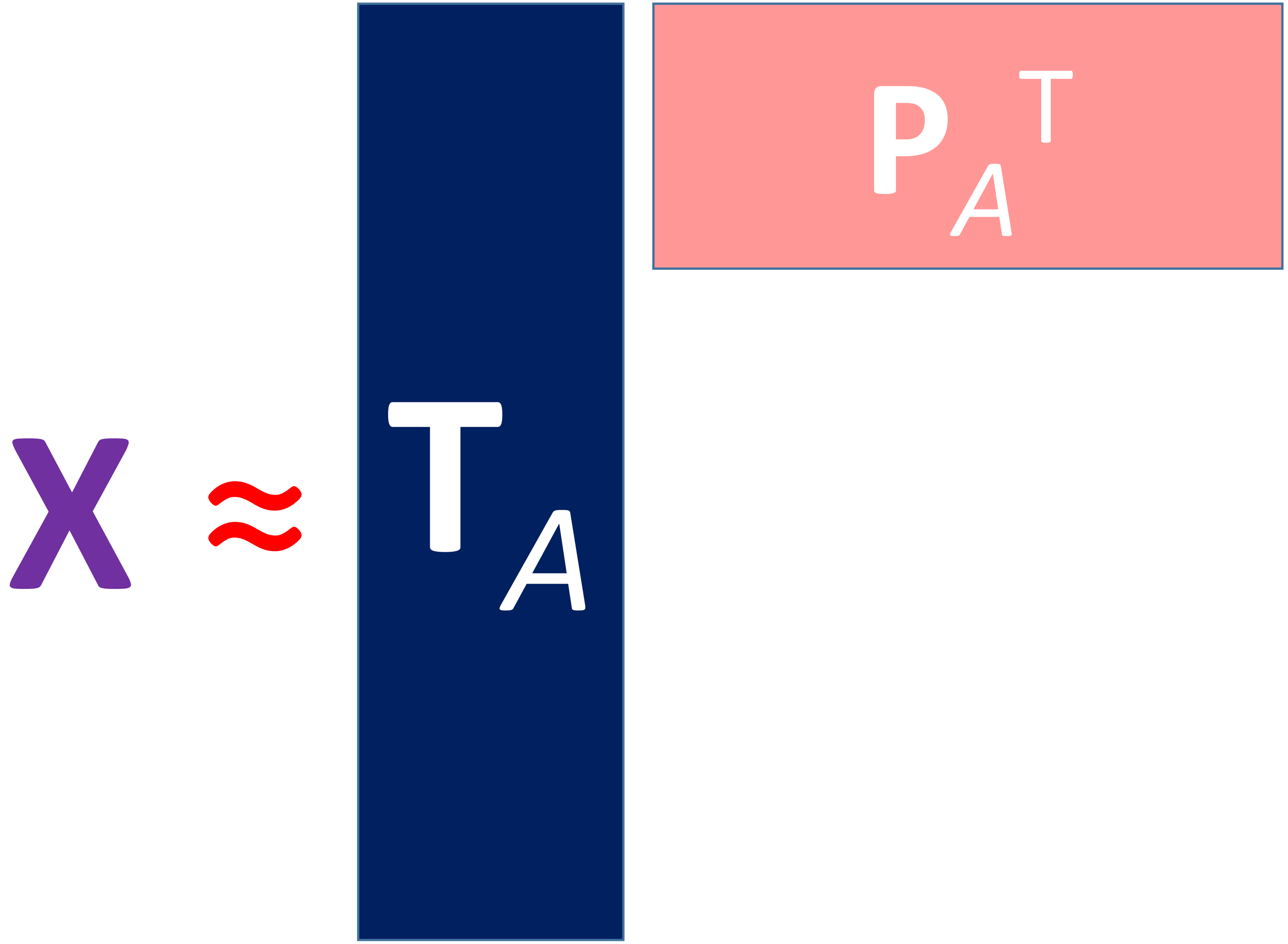


Principal component analysis

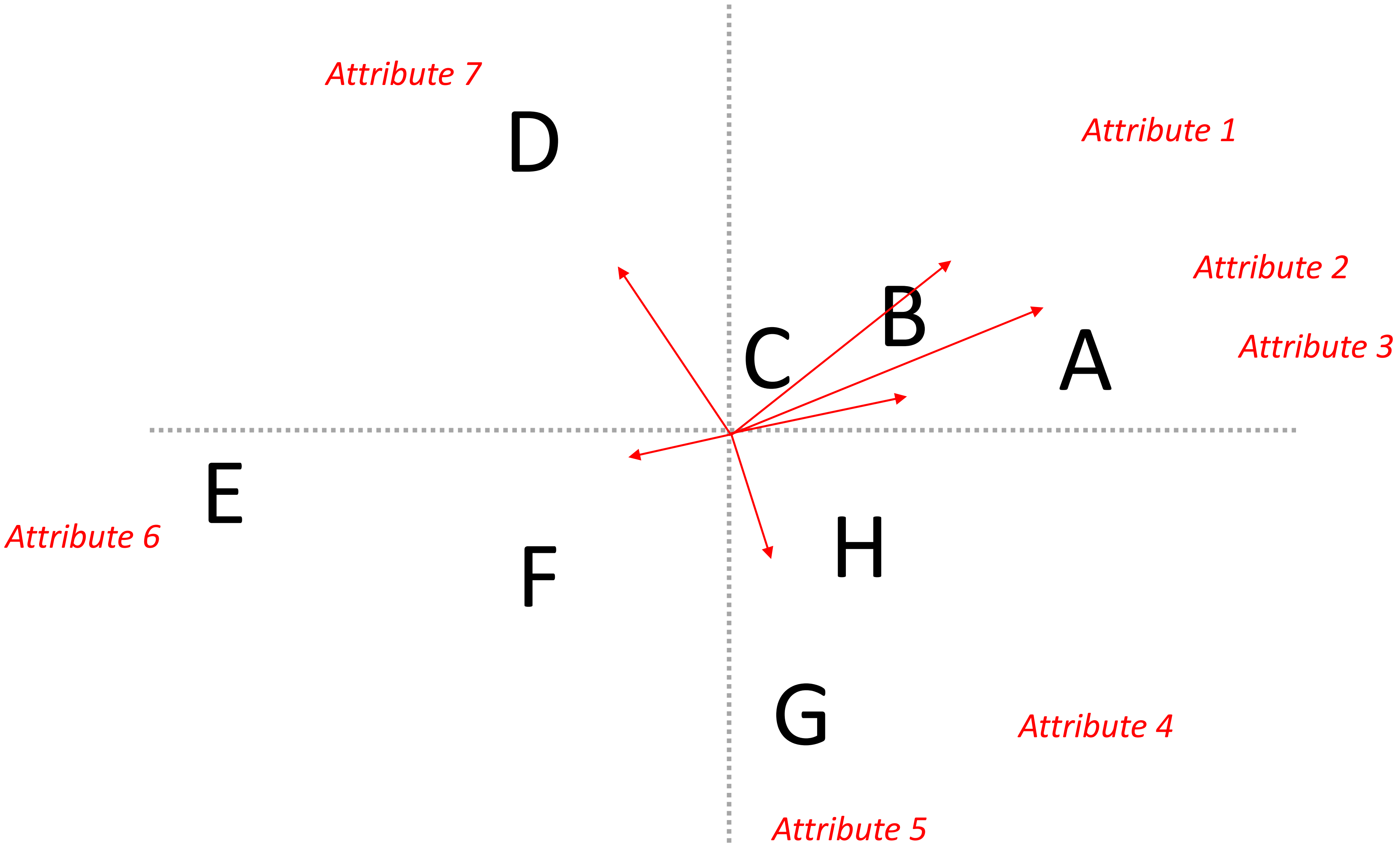


Dimension Reduction to *A* PCs

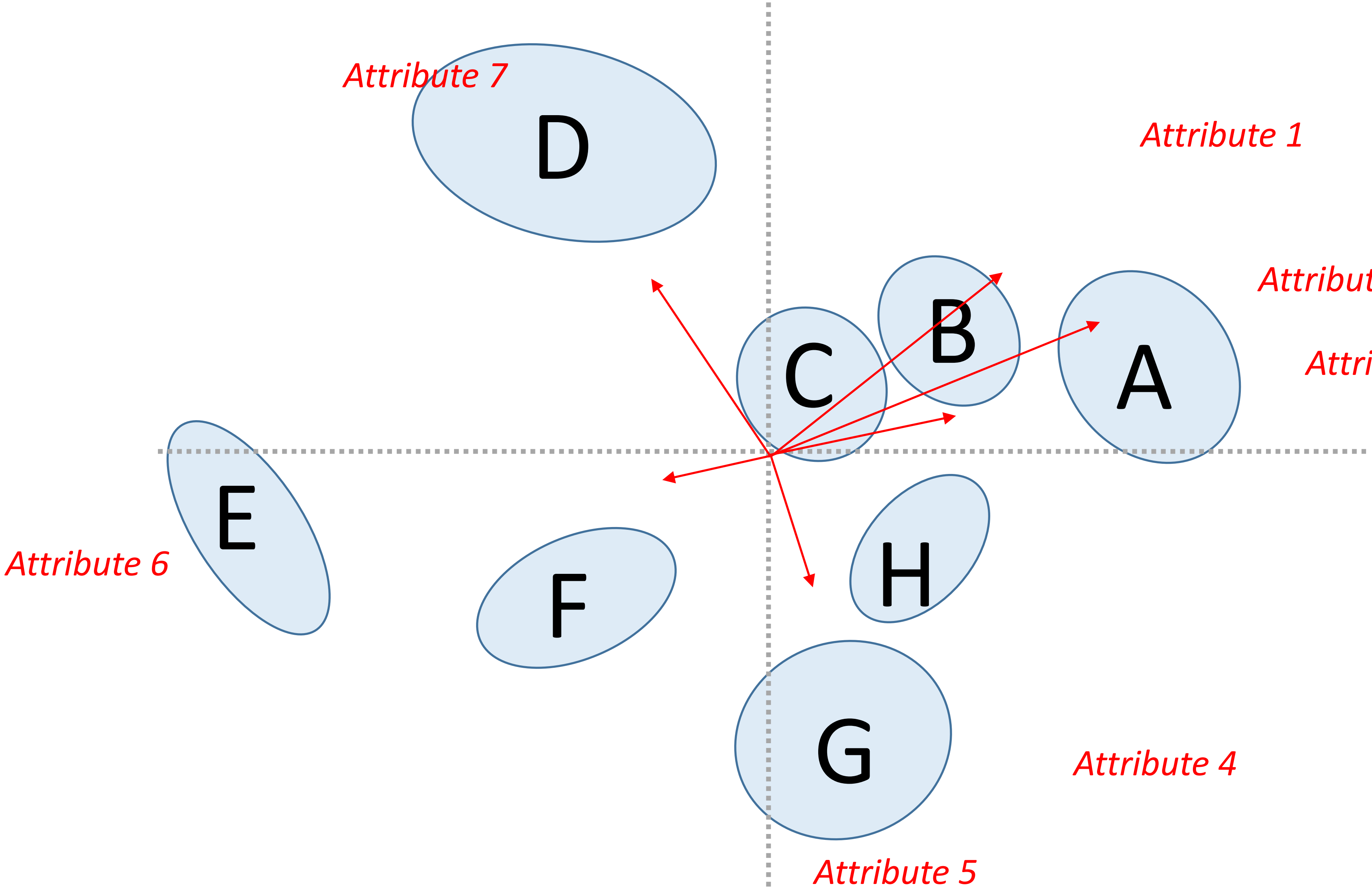
$$\mathbf{X} \approx \mathbf{T}_{A} \mathbf{P}_{A}^{\mathrm{T}}$$



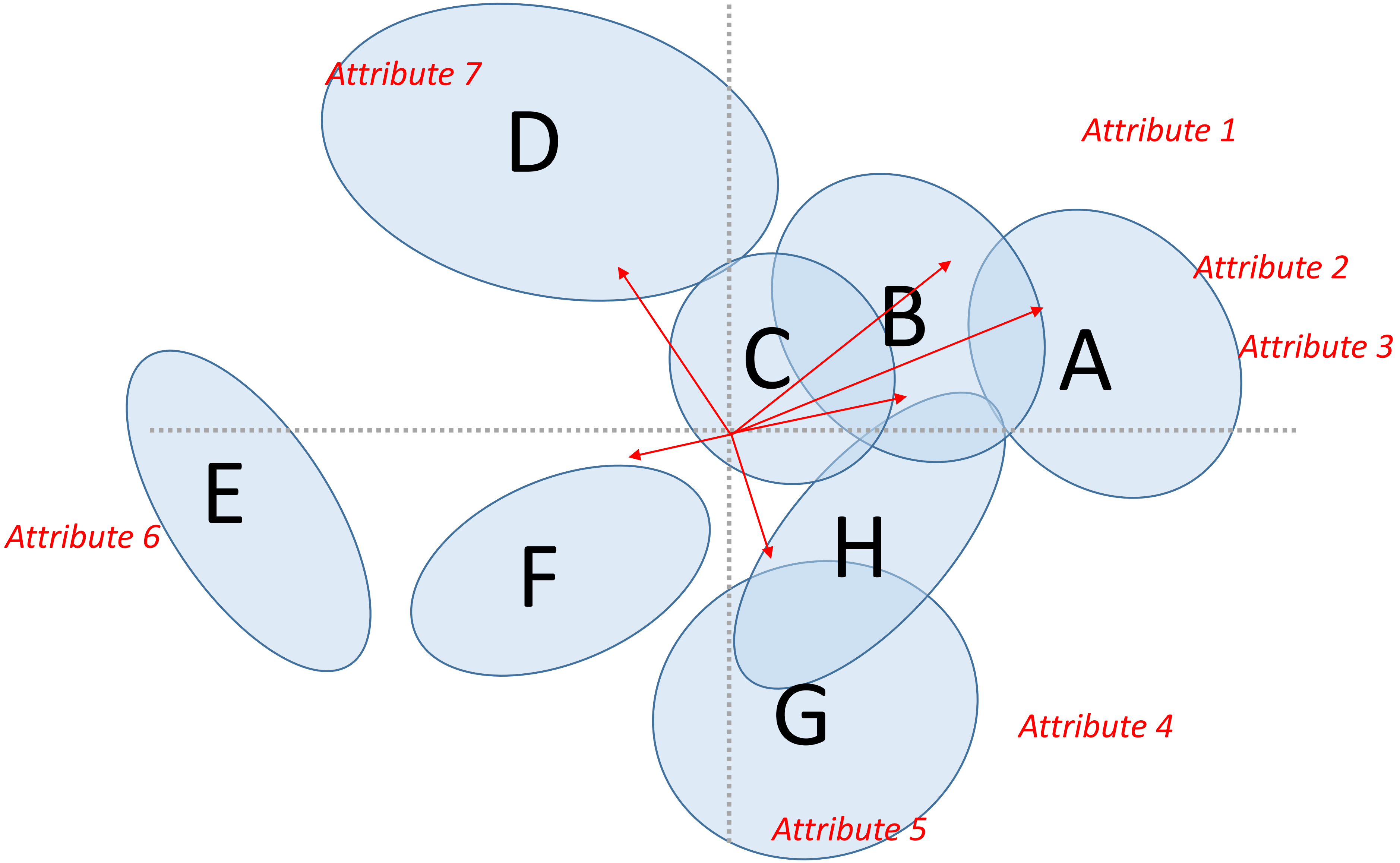
PCA results


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

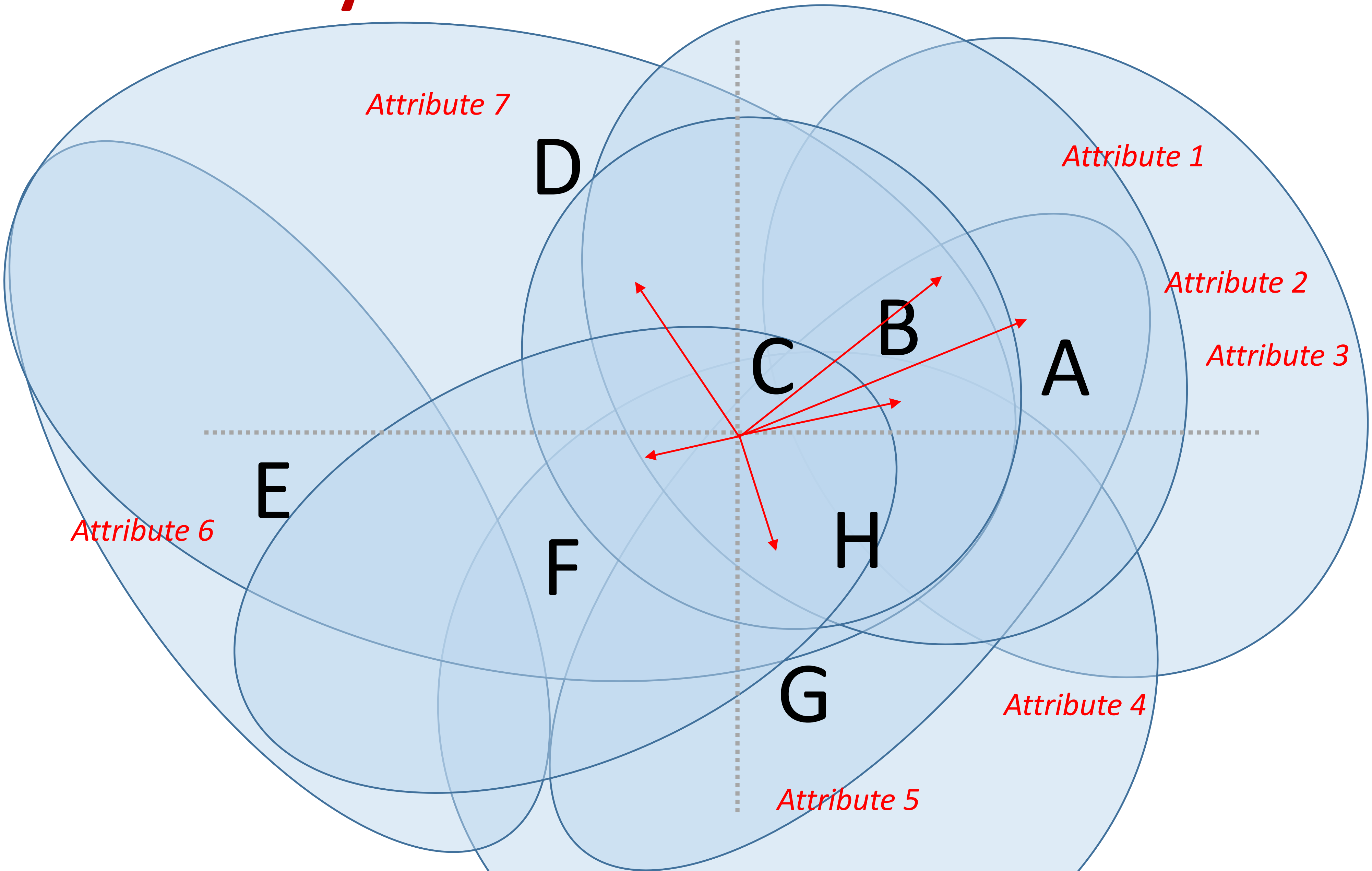
Uncertainty in PCA results



Uncertainty in PCA results



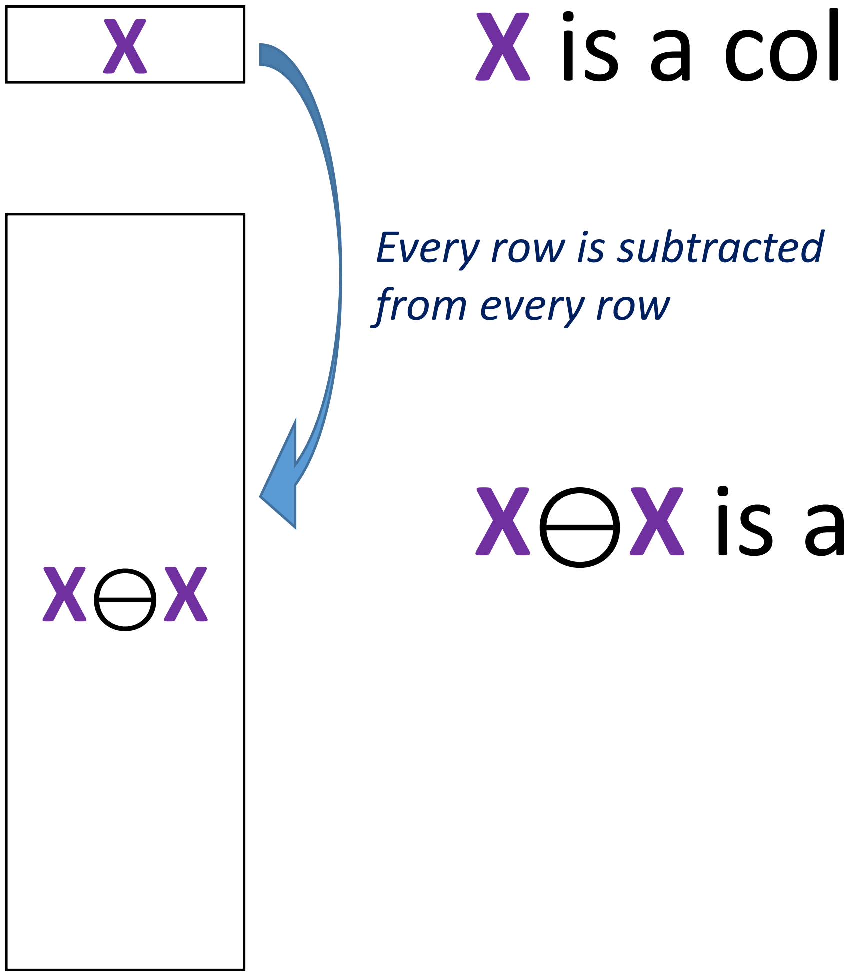
Uncertainty in PCA results



Paired Comparisons after PCA

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

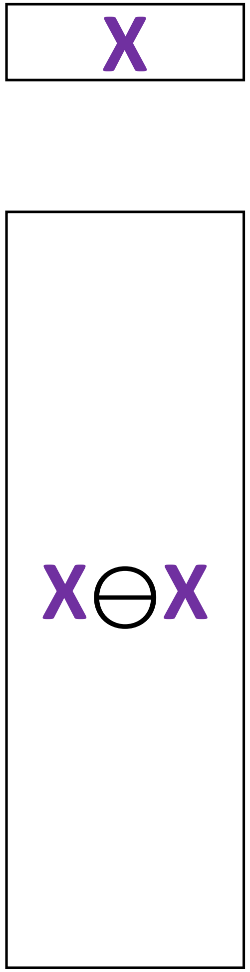
“Crossdiff-unfolding”



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

X⊖**X** is a column-centered ($J^2 \times M$) matrix

“Crossdiff-unfolding”



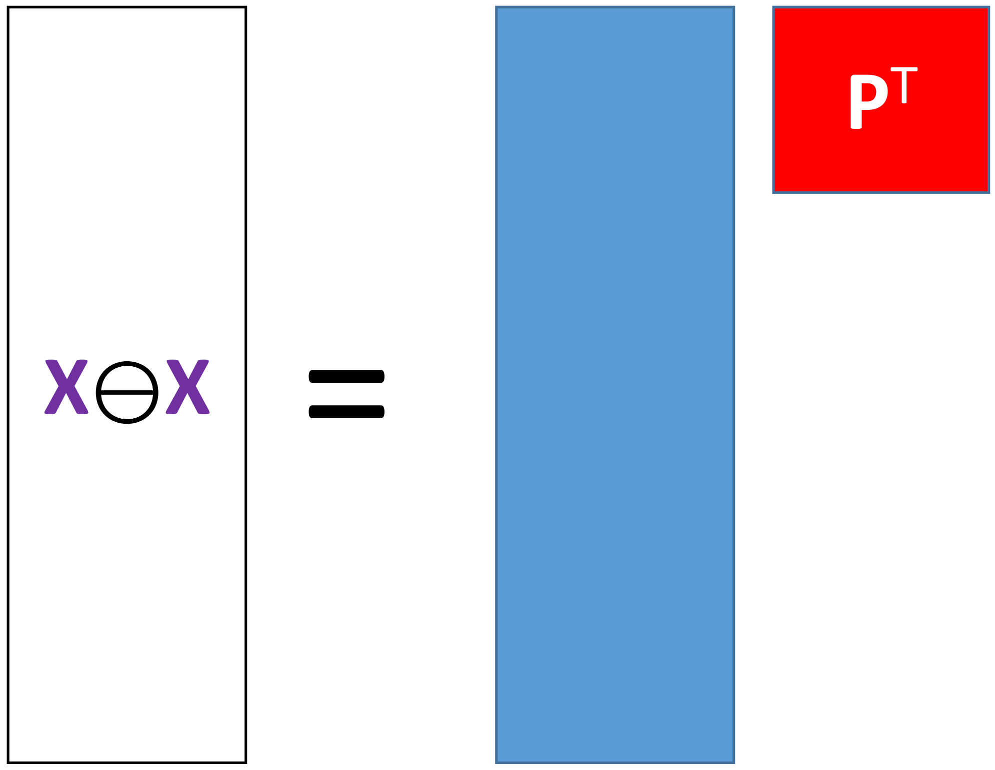
The covariance matrix of **X** and the covariance matrix of **X⊖X** are identical except for a multiplier.

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

Key relationships

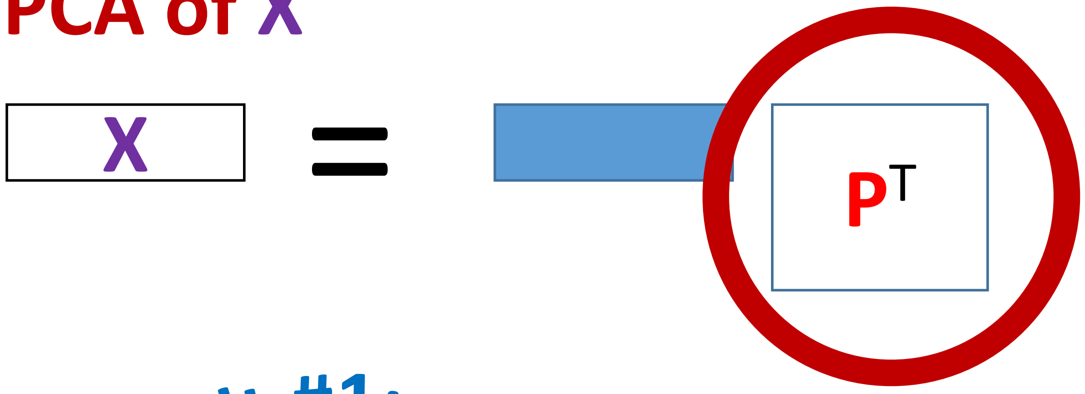
PCA of X

PCA of X⊖X

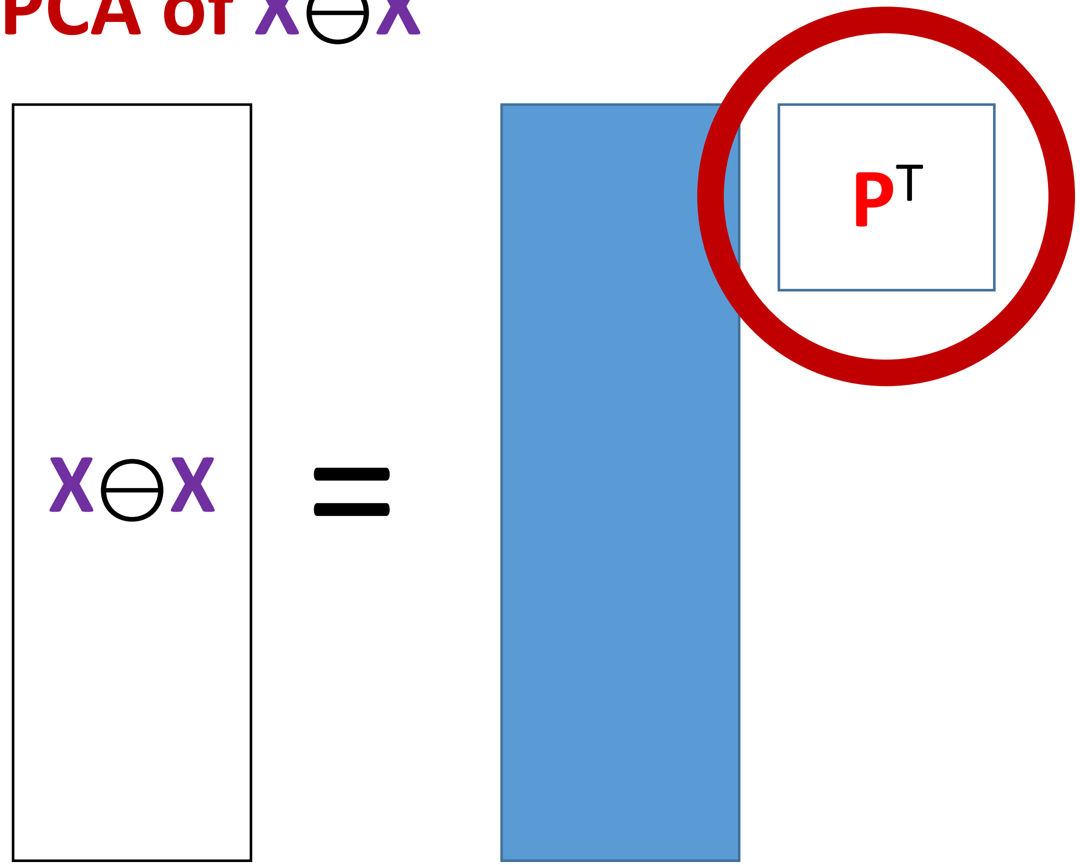


Key relationships

PCA of X



PCA of $X \ominus X$

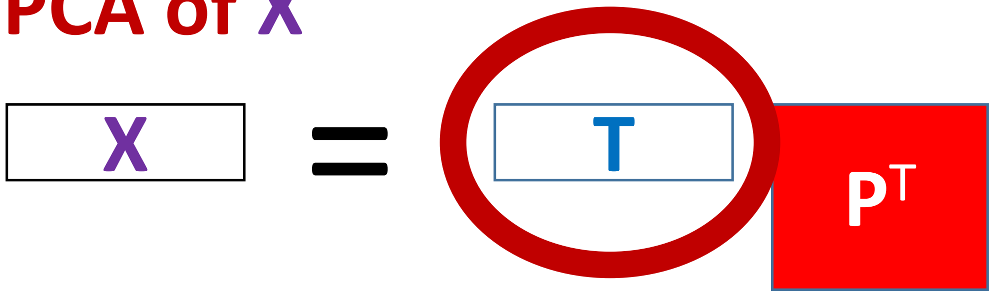


Key result #1:

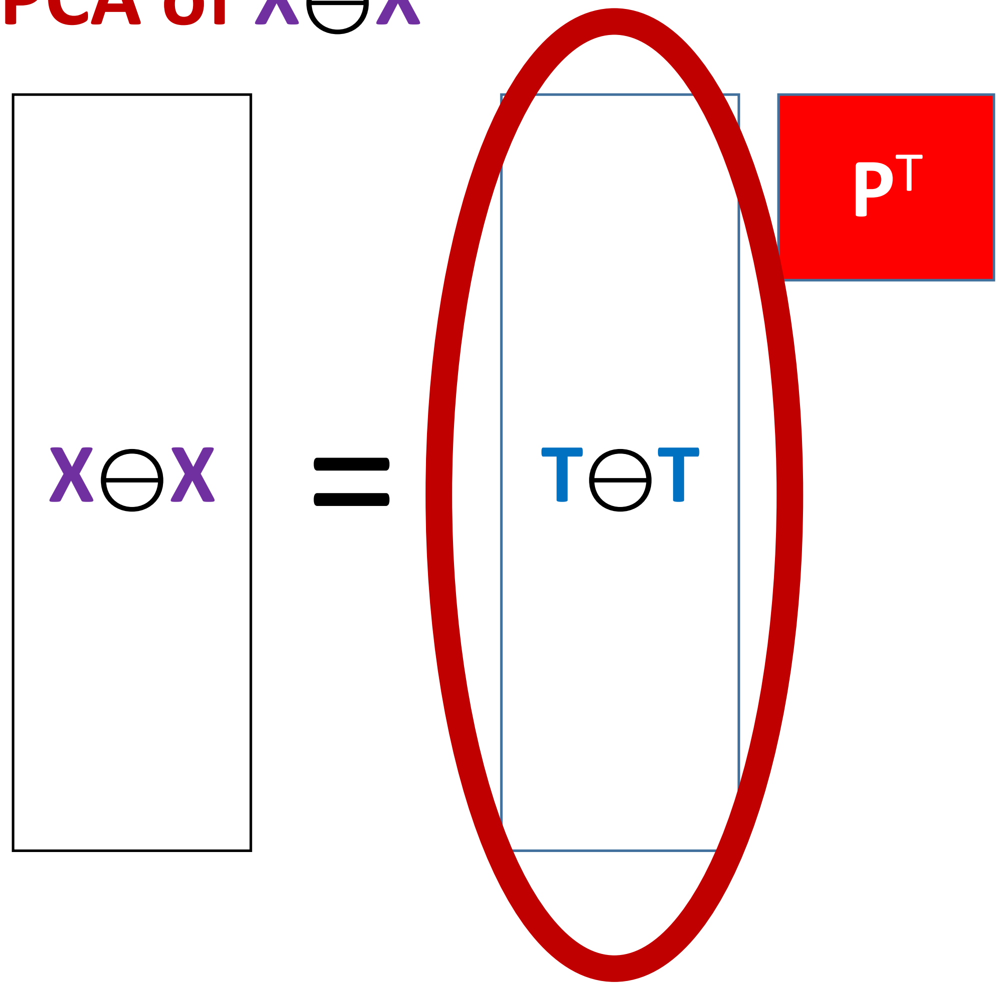
Loading matrices obtained from these two PCA solutions are identical.

Key relationships

PCA of X



PCA of $X \ominus X$



Key result #2:

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

Paired comparisons

Row objects in **X** *and* **all paired comparisons** have the same PCs

Uncertainty in Paired Comparisons after PCA

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

The uncertainty cloud of each paired difference **accounts for mutual dependencies** and can be used to obtain…

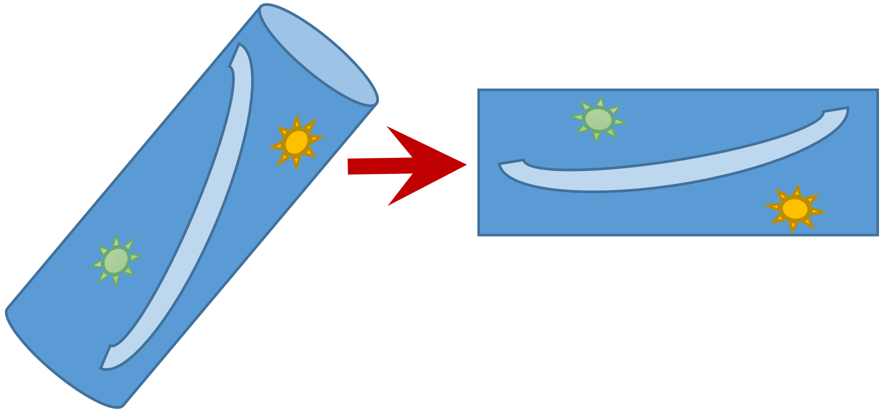
nonparametric uncertainty regions

confidence ellipsoid approximations

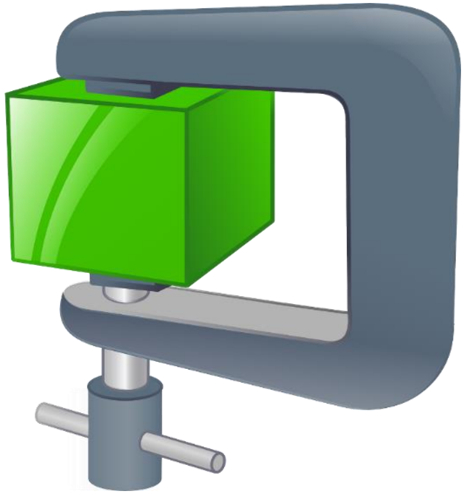
P values

Principal component analysis

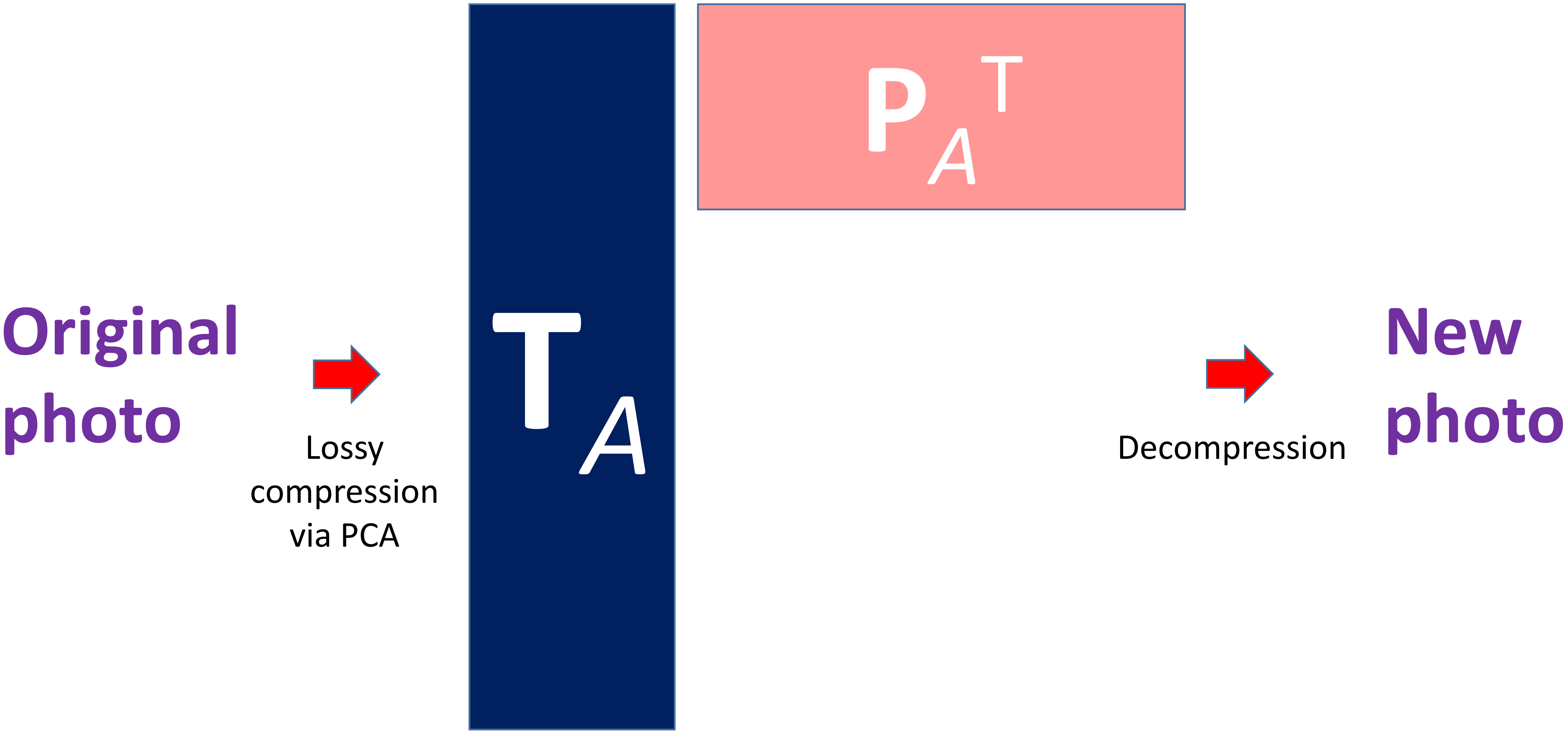
PCA is a statistical method that maximizes the variance in the standardized linear projection of a matrix.



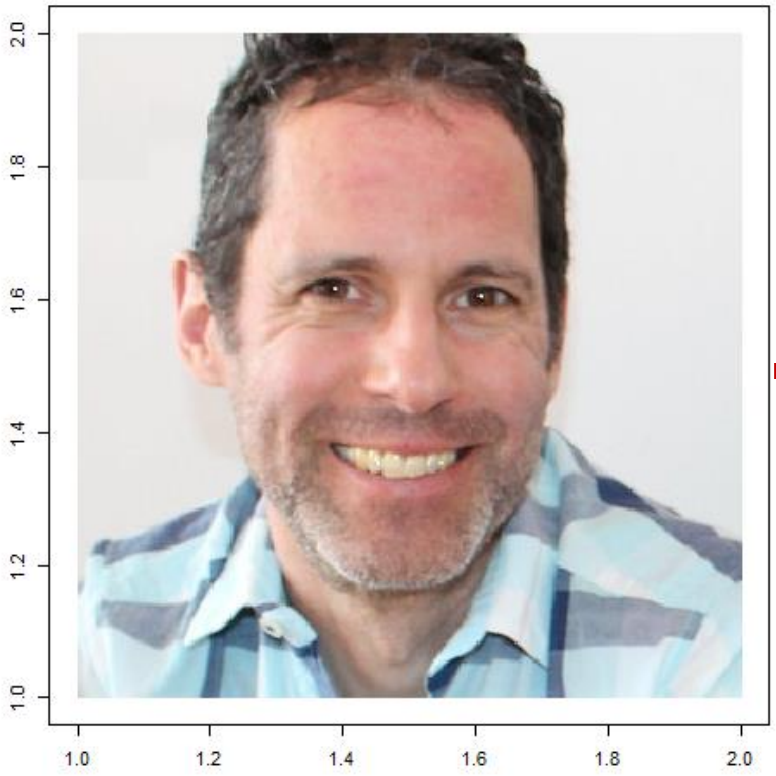
PCA is a method for **data compression** via dimension reduction.



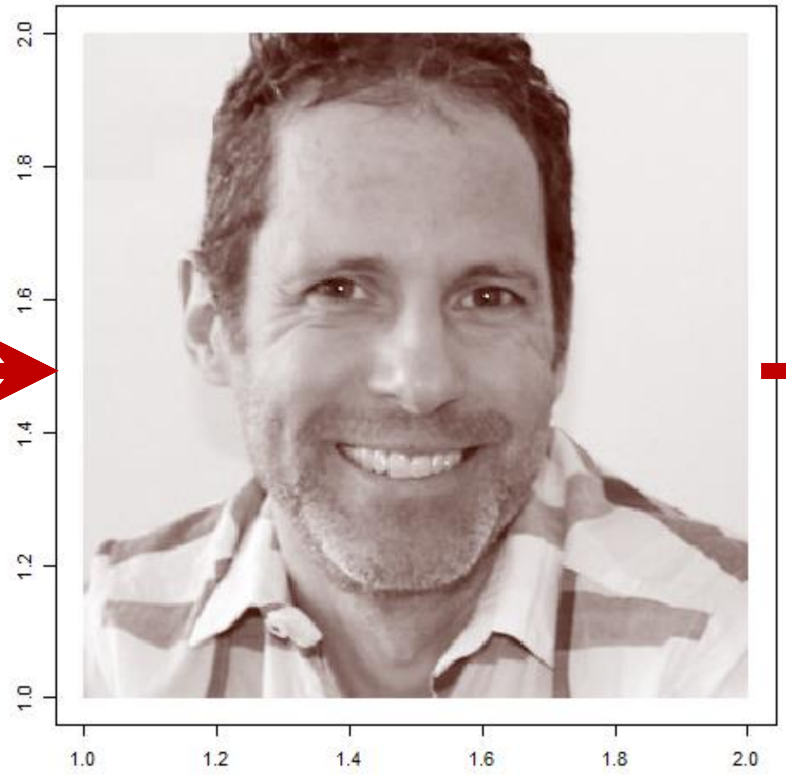
PCA of a Photograph



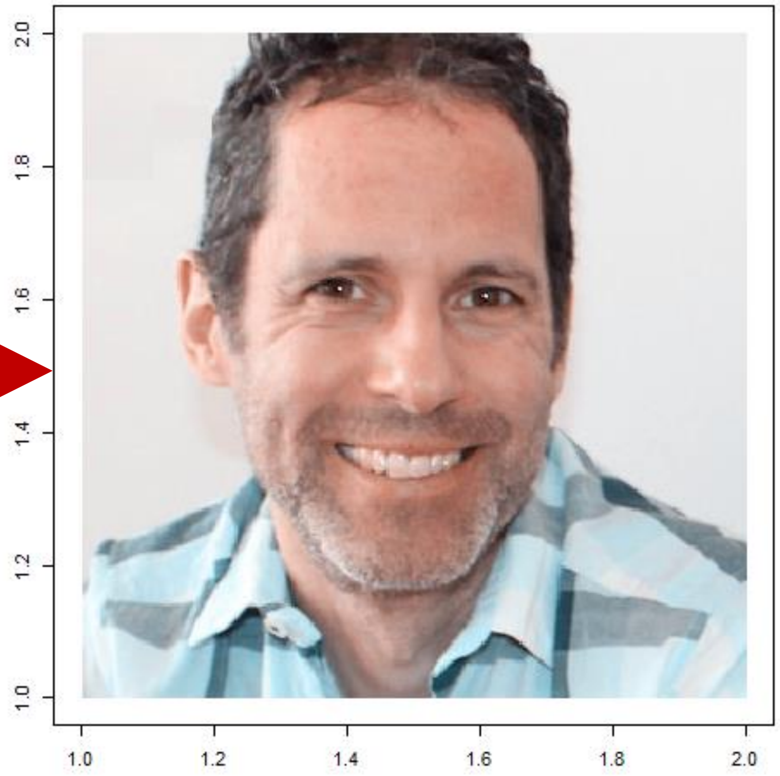
Lossy compression – example 1



Original image
has 3 components (RGB)

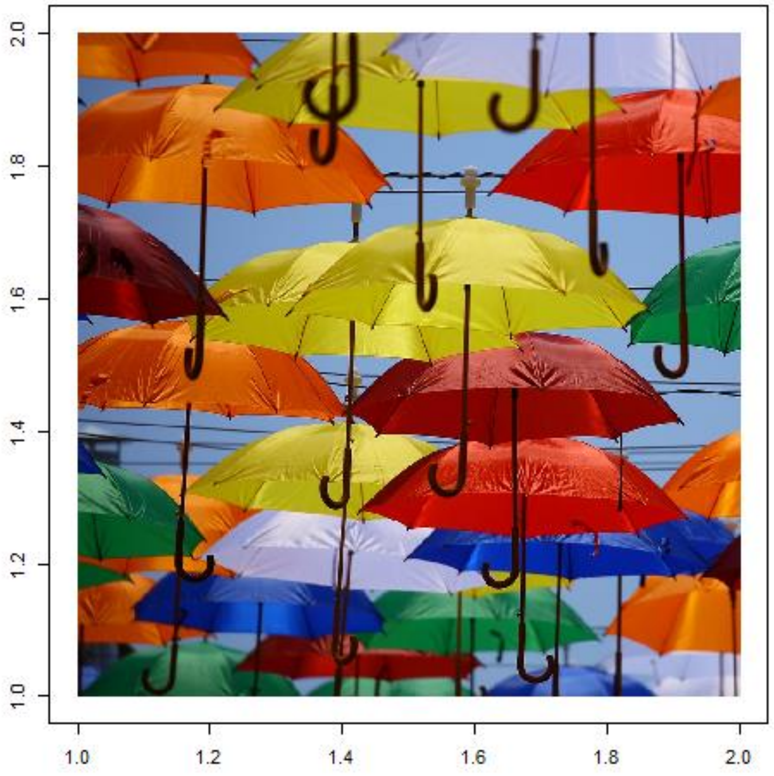


Compression to 1 PC
93% of RGB variance
extracted

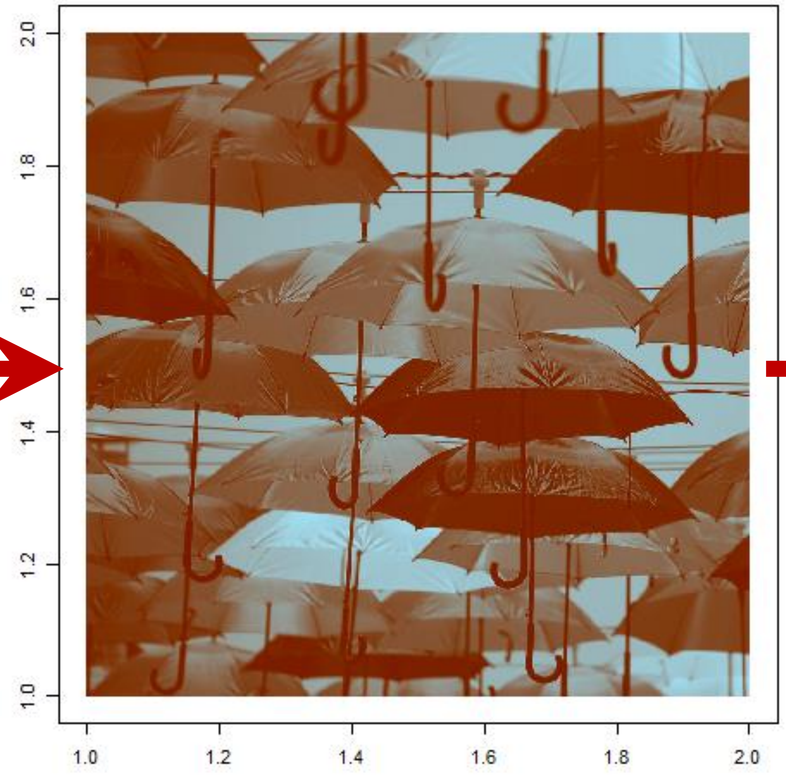


Compression to 2 PCs
97% of RGB variance
extracted

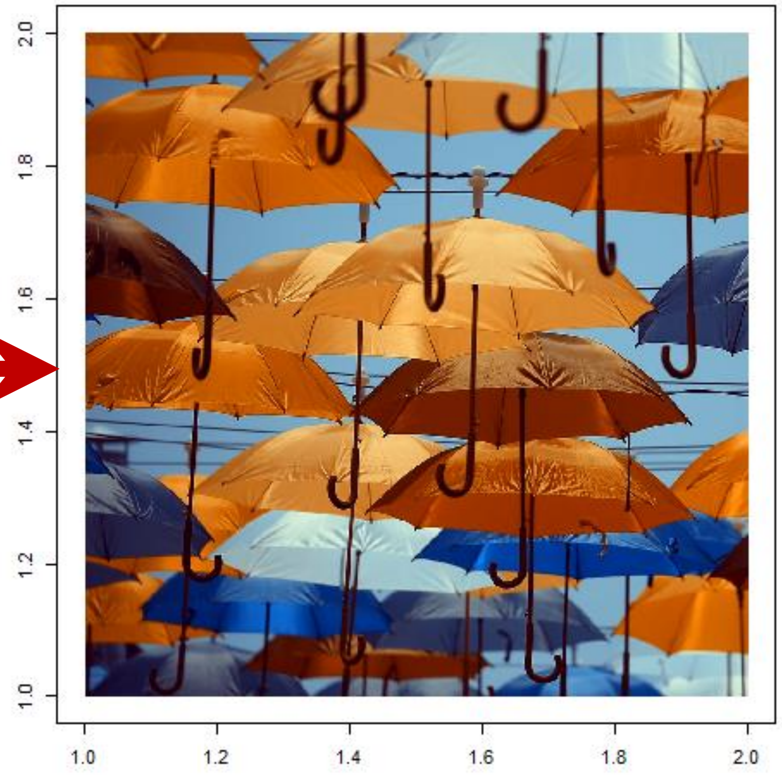
Lossy compression – example 2



Original image
has 3 components (RGB)



Compression to 1 PC
57% of RGB variance
extracted



Compression to 2 PCs
92% of RGB variance
extracted

Investigating a Subset of Paired Comparisons after PCA

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

When are only a subset of paired comparisons relevant?

Examples:

1. **Many Test Products *vs* One Control**

   Focus on Test-Control pairs,
   not Test-Test pairs

2. **Temporal sensory data**

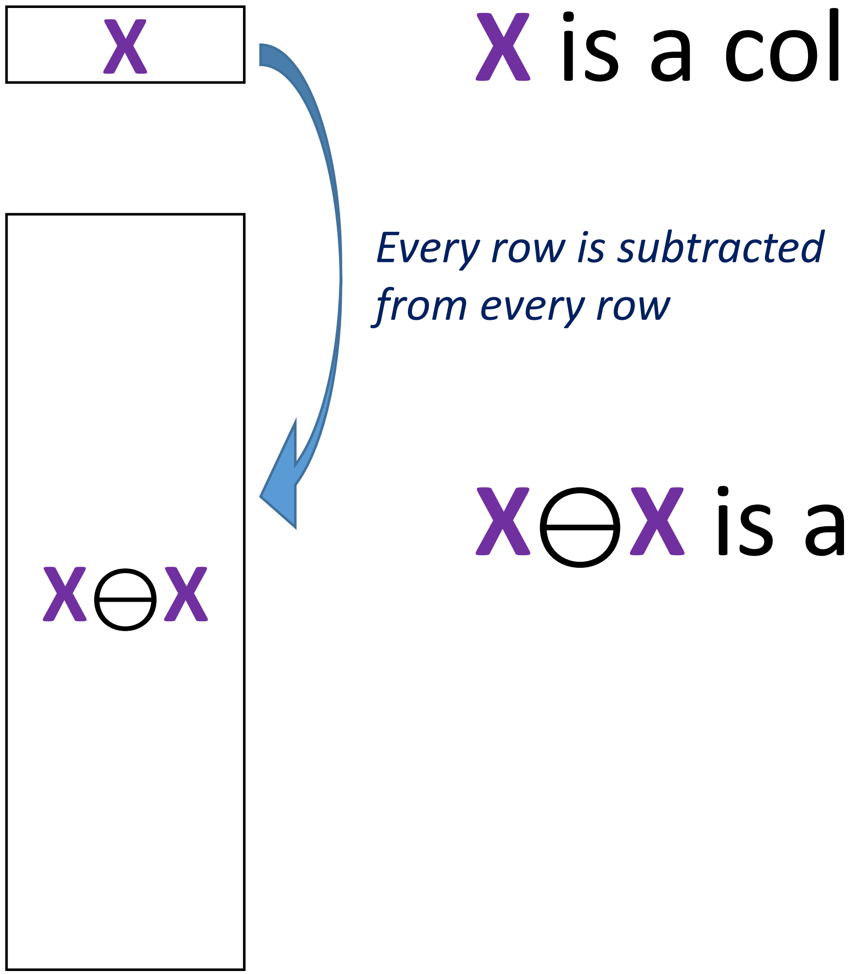
   Focus on Within-timepoint pairs,
   not Across-timepoint pairs

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.

Crossdiff-unfolding



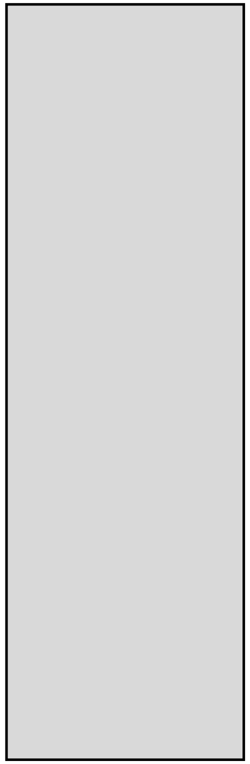
X is a column-centered $(J \times M)$ matrix

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

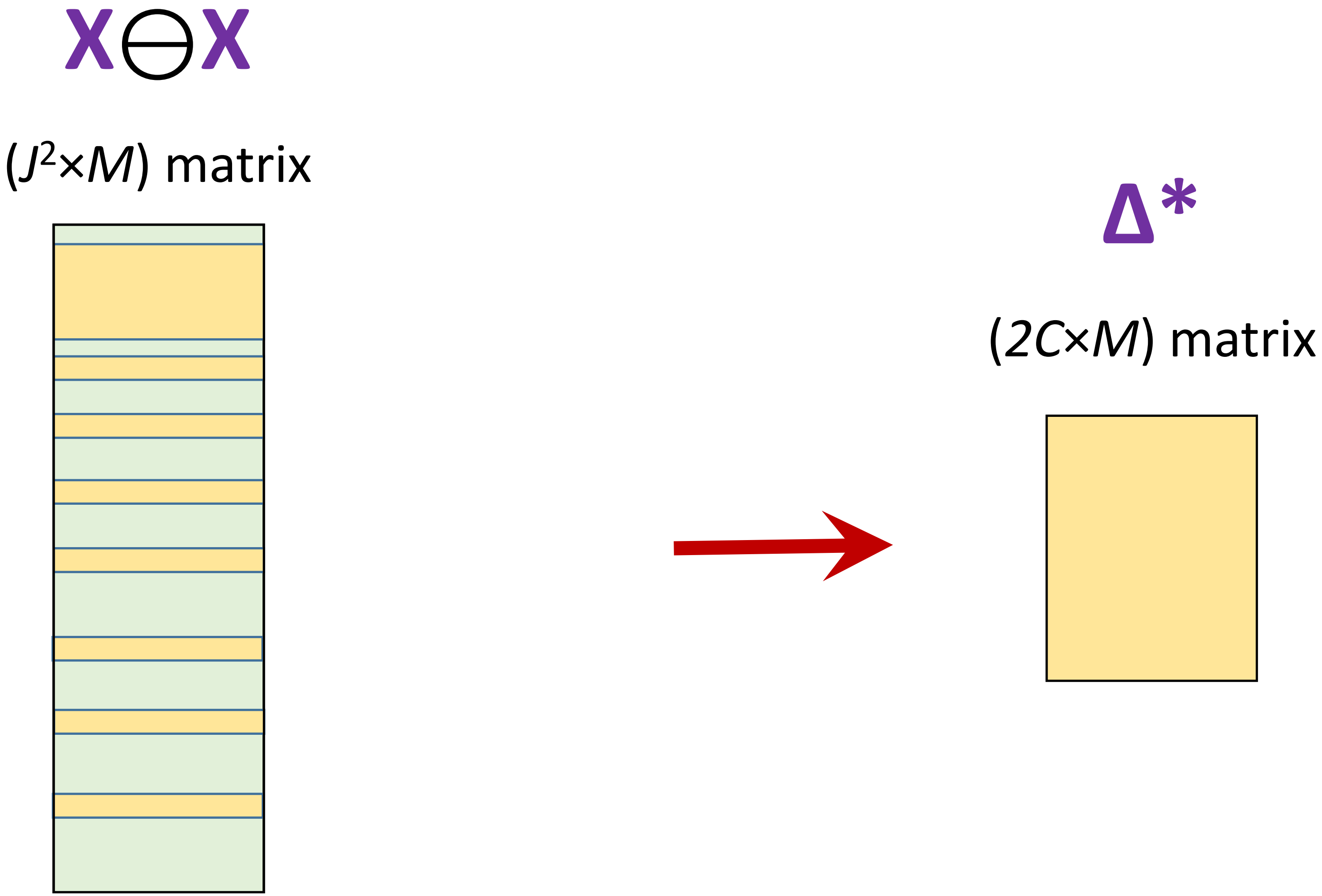
Rows of $\mathbf{X} \ominus \mathbf{X}$ contain all paired comparisons

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

($J^2 \times M$) matrix

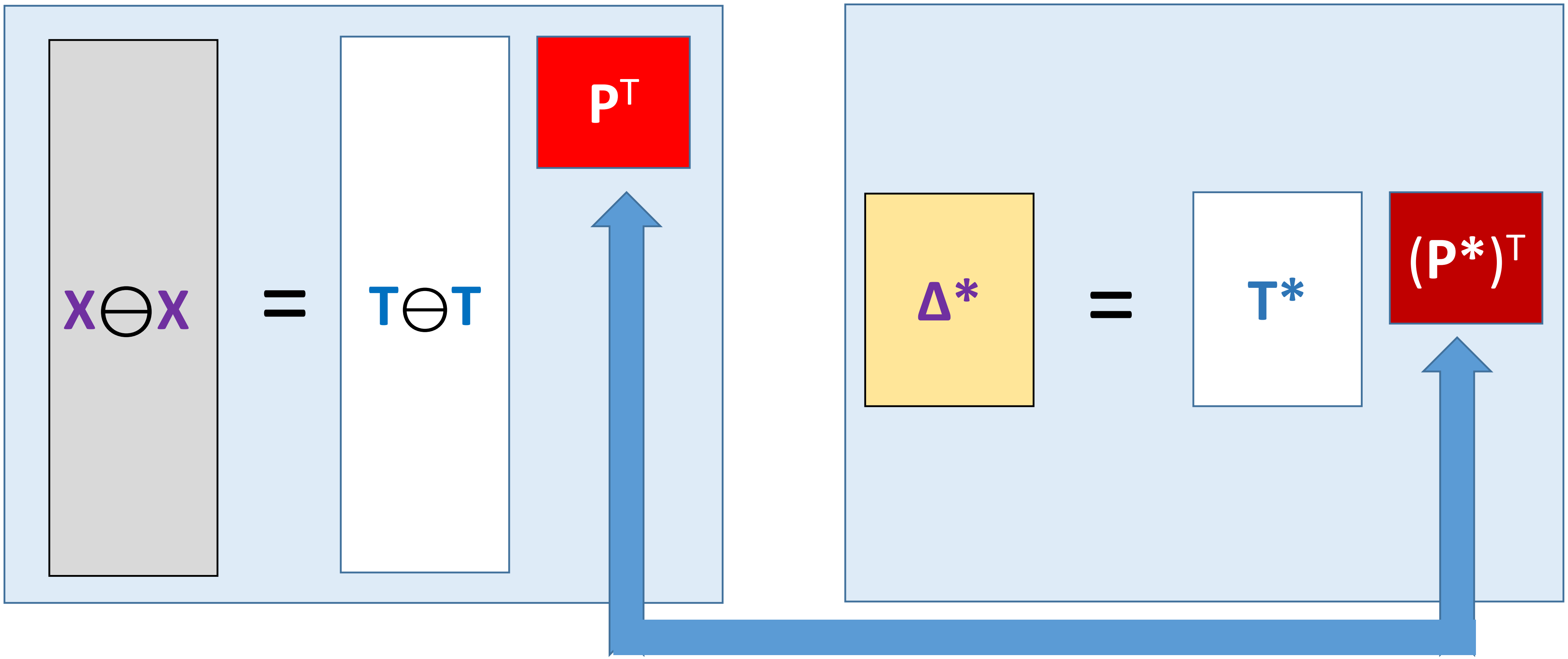


Matrix Δ* contains only *C* relevant paired comparisons



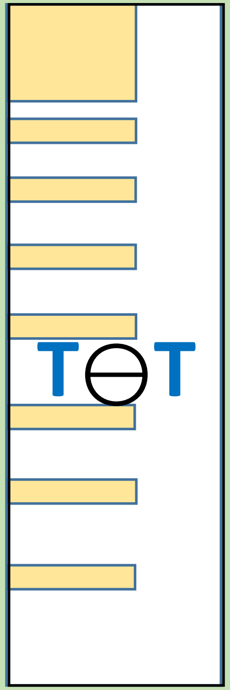
Δ* contains a subset of the rows in X⊖X

PCs of X⊖X and PCs of Δ* are usually different

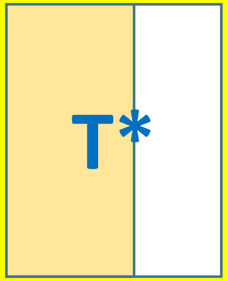


Calculate the relevant sum-of-squares extracted

Sum of squares of **relevant rows** in *A* PCs

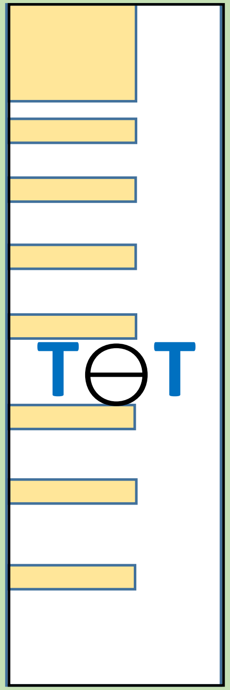


Sum of squares of **all rows** in *A* PCs

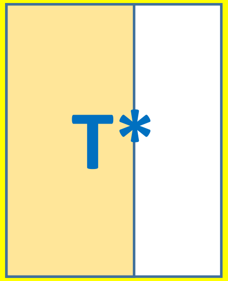


Gain of focusing on *A* PCs of Δ* instead of *A* PCs of X⊖X

Sum of squares of **relevant rows** in *A* PCs



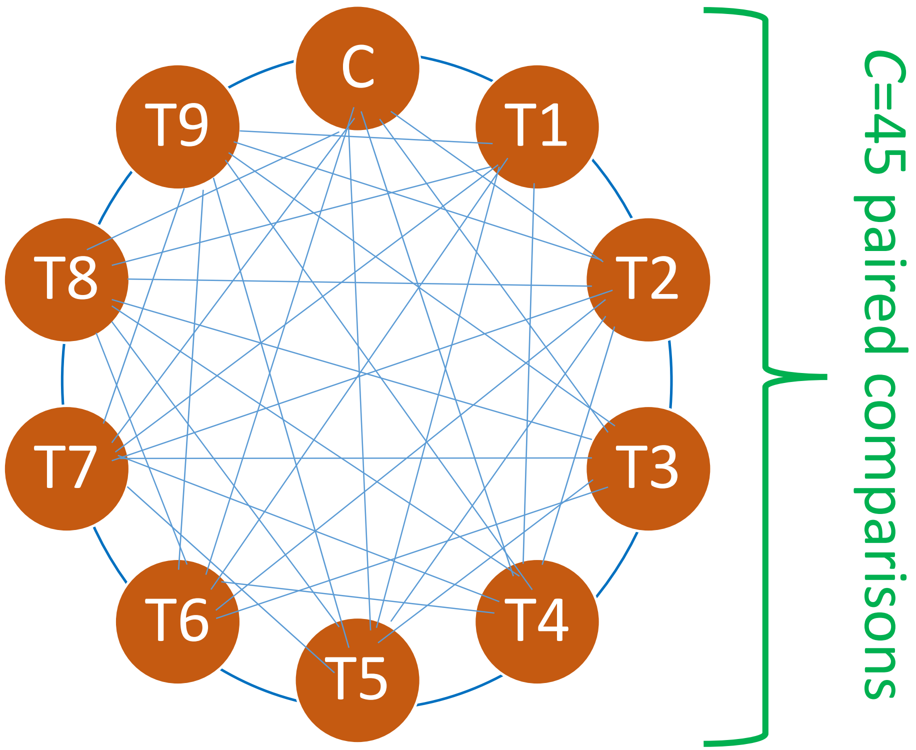
Sum of squares of **all rows** in *A* PCs



Gain = 100(/ - 1)%

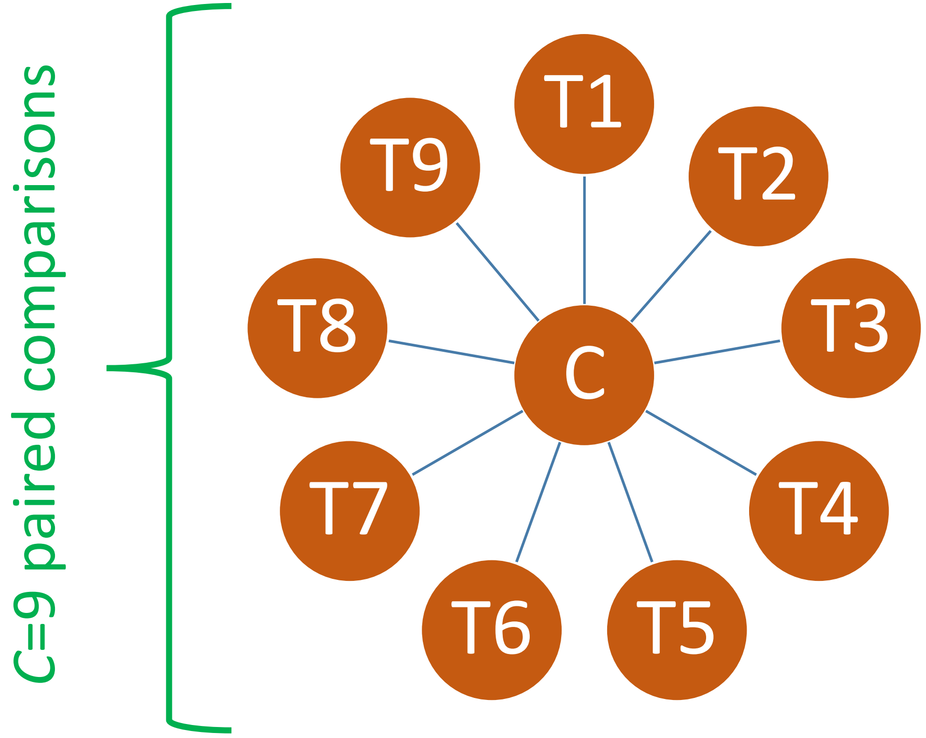
Example 1. QDA of multiple products vs a control

All Paired Comparisons



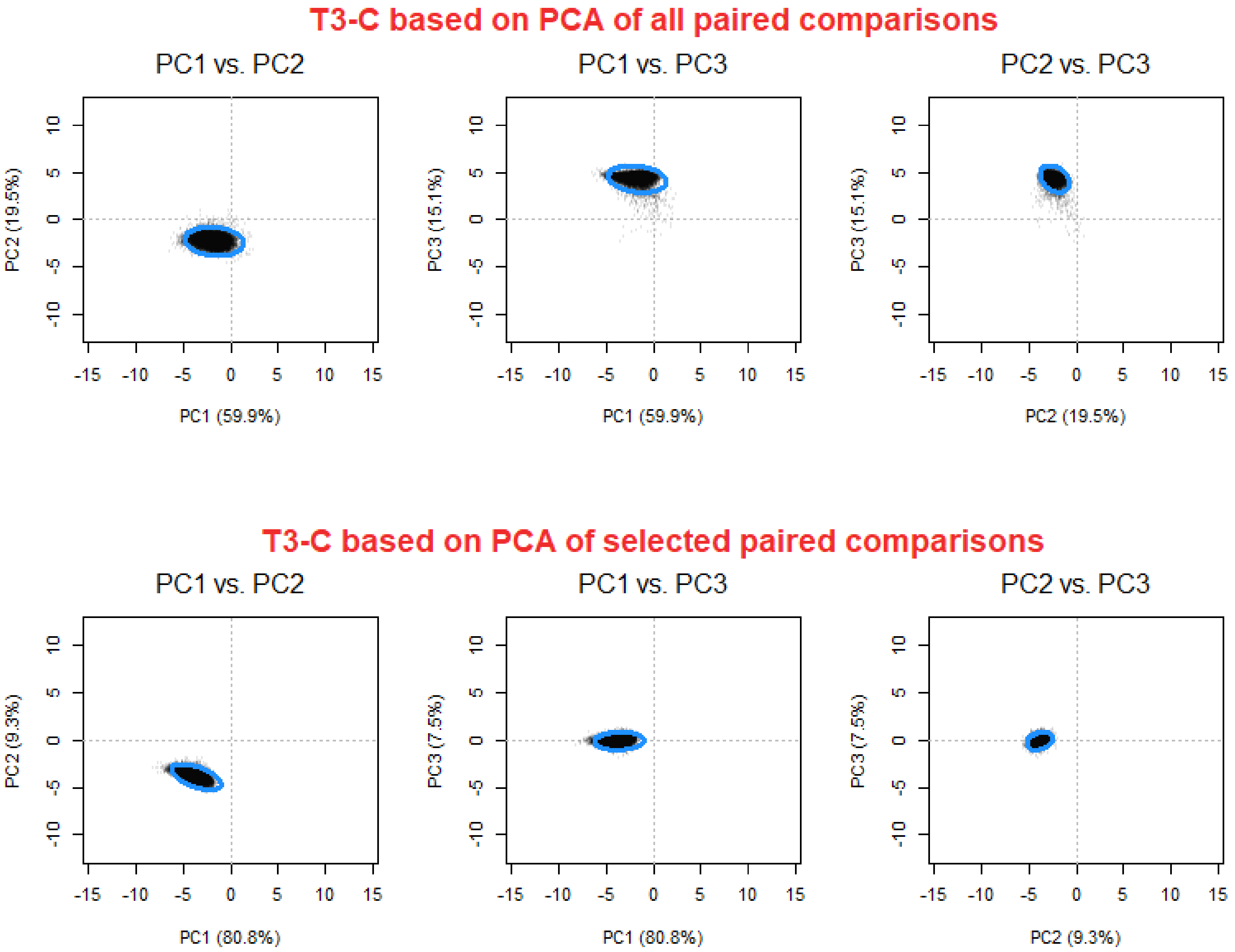
$\mathbf{X} \ominus \mathbf{X}$ has $J^2=100$ rows

Relevant Paired Comparisons



$\boldsymbol{\Delta}^*$ has $2C=18$ rows

Example 1. QDA of multiple products vs a control



Gain:

1 PC:
15%

2 PCs:
14%

3 PCs:
1%

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

Example 2. Temporal check-all-that-apply

All Paired Comparisons

- 8 yogurts × 56 timepoints
- 448 combinations
- All pairs = 100,028
- 10 attributes

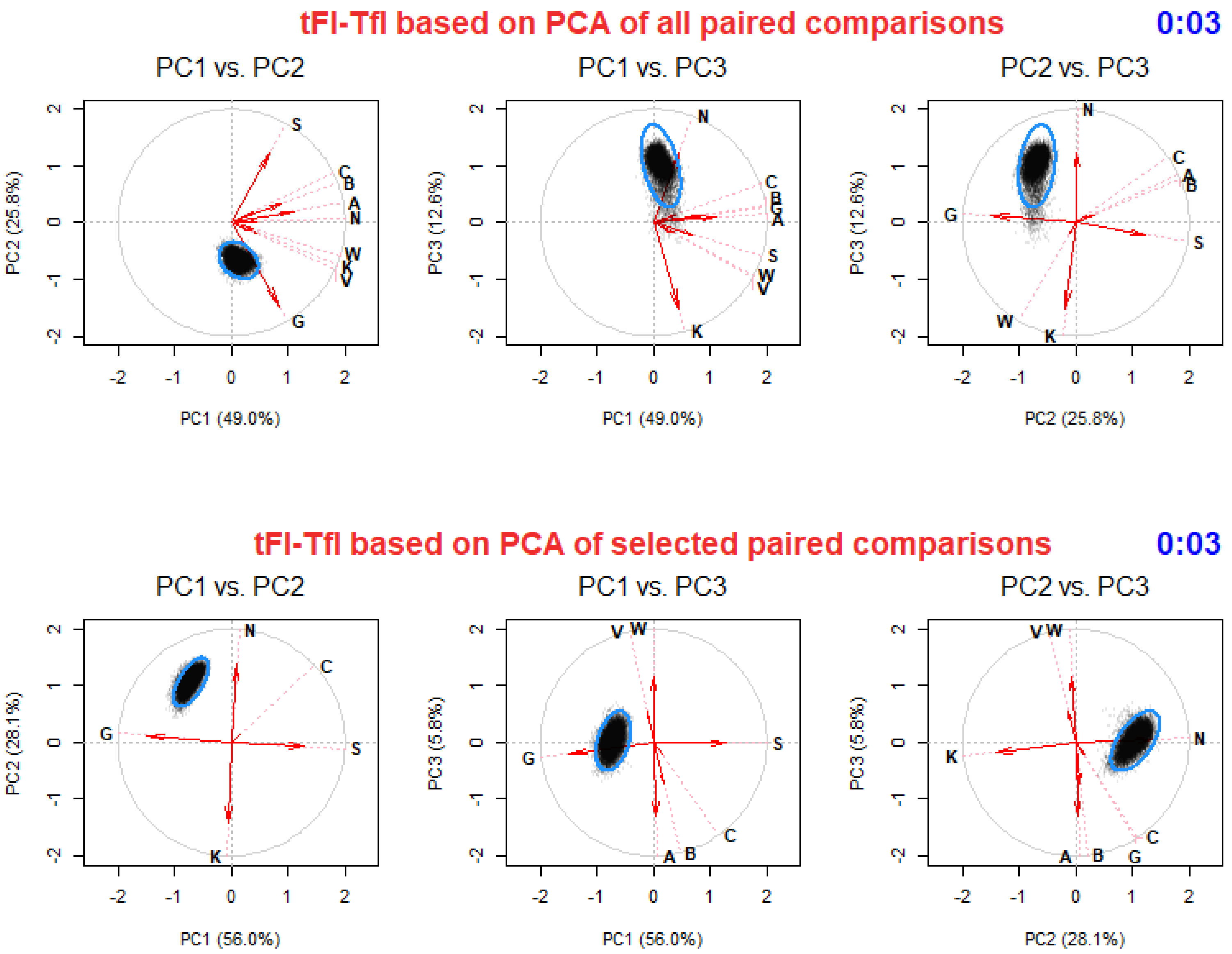
X⊖X has dimension
100028 × 10

Relevant Paired Comparisons

- 28 within-timepoint pairs
- 56 timepoints
- C = 28×56 = 1568
- 10 attributes

Δ* matrix has dimension
3136 × 10

Example 2. Temporal check-all-that apply



Gain:

1 PC: **>3500%**

2 PCs: **52%**

3 PCs: **1%**

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

When only a subset of paired comparison are relevant

Advantages of PCA of Δ* over PCA of X⊖X

- Δ* contains only relevant variance

  …so ***all*** variance extracted by PCA of Δ* is relevant
- Important PCs will tend to have large %VAF
- More natural to focus interpretation on PCs with large %VAF
- Recommended only if a subset of paired comparison are relevant

Advantages of PCA of X⊖X over PCA of Δ*

- Interpretations identical to interpretations of PCA of X
- Conventional so easier to communicate
- Row objects in X are well represented in PCs of X⊖X

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