In Pursuit of the "Golden Curve"

A Comparison of Functional Data and Partial Least Squares Analyses on Serial Data

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Introduction

Introduction to the serial / curve sensor data collected and some of the many questions posed.

Understanding K-data curves and linking them to *Yield 1 (smaller is better)*:

- Use of Functional Data Analysis (FDA) to assess this link.
- More traditional modelling via Partial Least Squares (PLS) – analysed using SIMCA
- Common links between the two methods.

Linking P-data curves to *Yield 2 (larger is better)*:

- Making use of some tools in SIMCA for exploratory data analysis and modelling.
- Use of FDA.

Summary and next steps.

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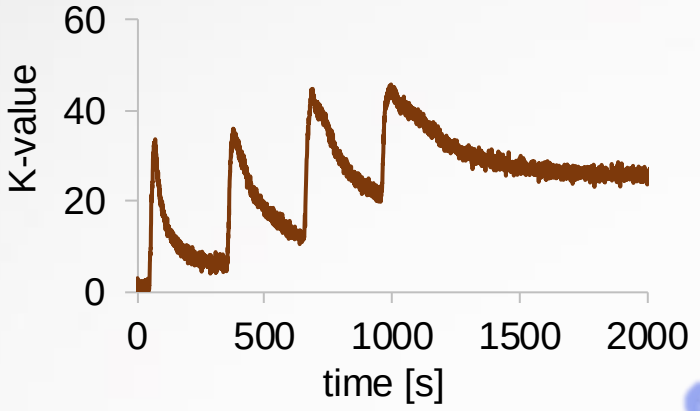
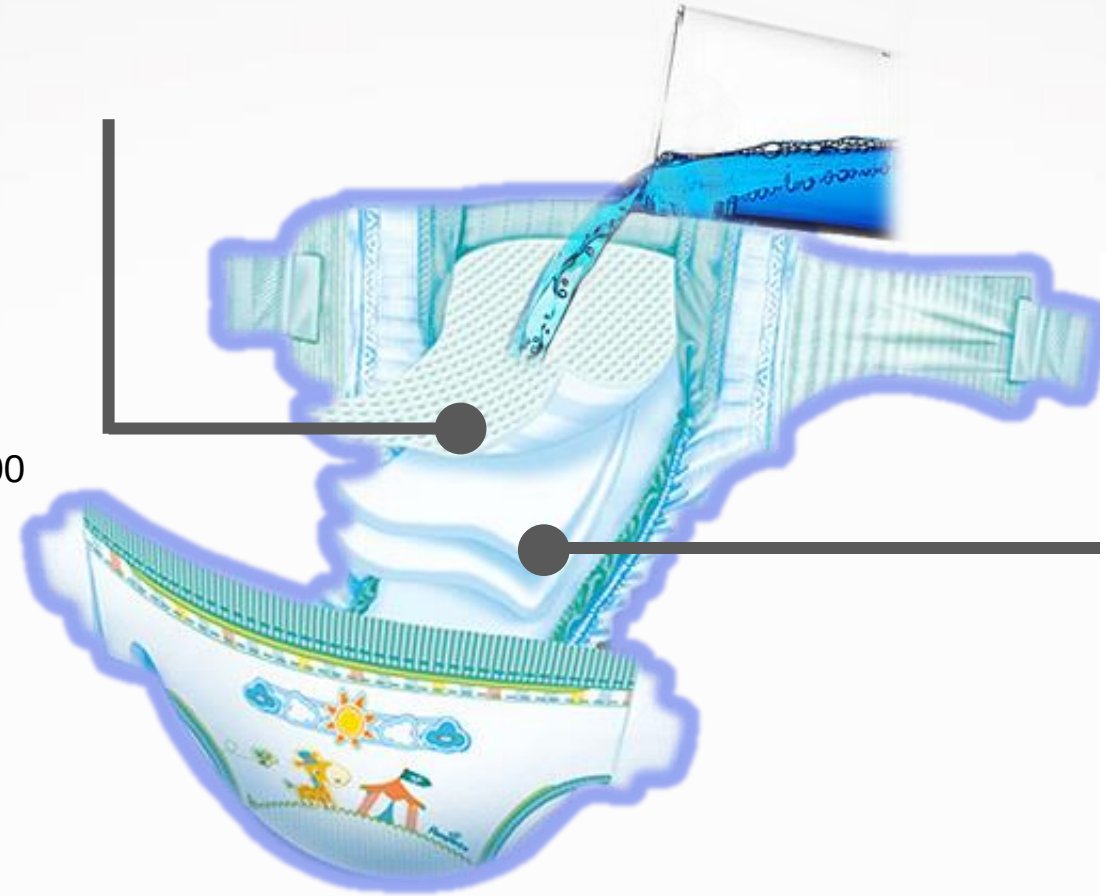
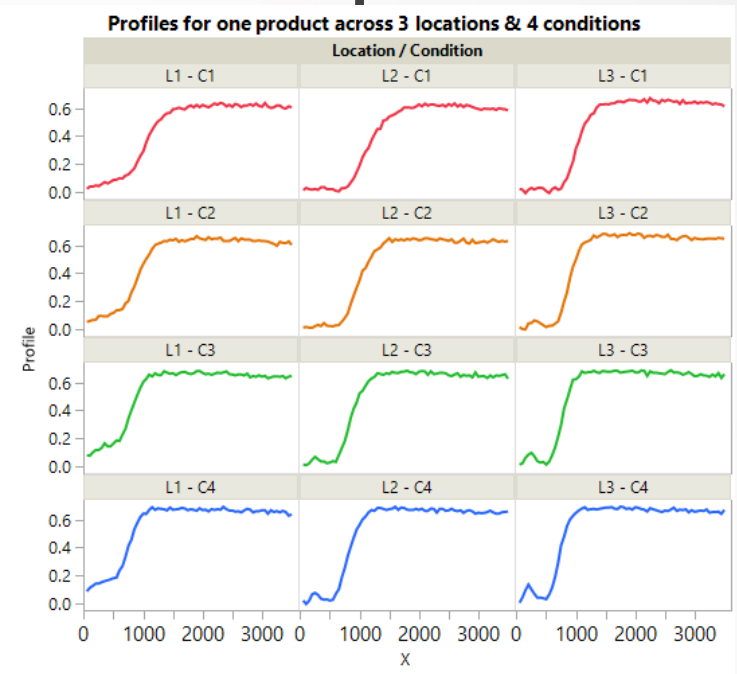
ANALYTICAL

K-data curves





P-data profiles



3 replicates for each endpoint measured

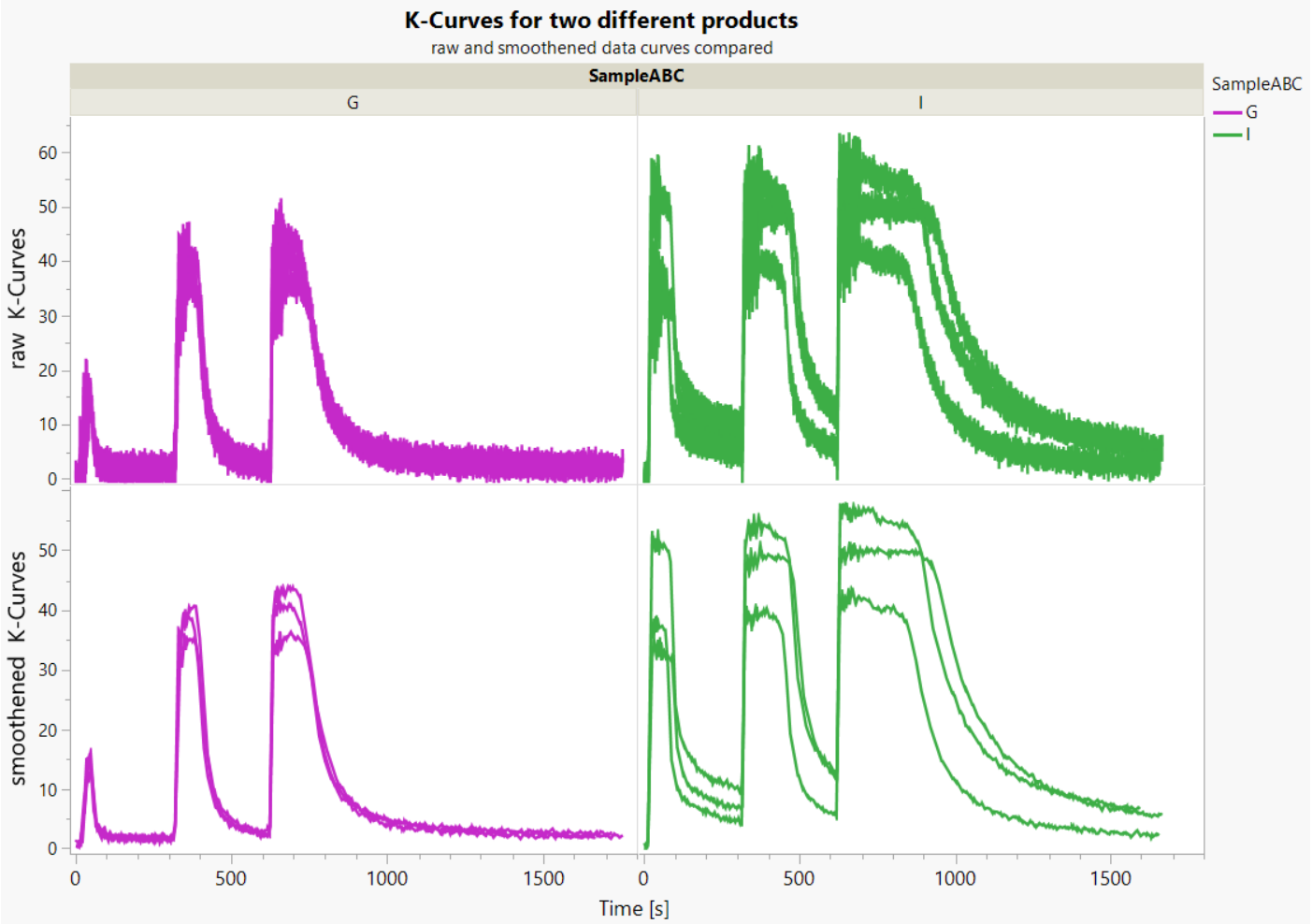
K-data

K-data quite oscillating / noisy due to the very high frequency at which they are measured

Smoothing indicated prior to fitting

Moving Average with “Local width” = 20s used

Curves / derivatives not smooth. FDA analyses smooth curves usually!



FDA Demo

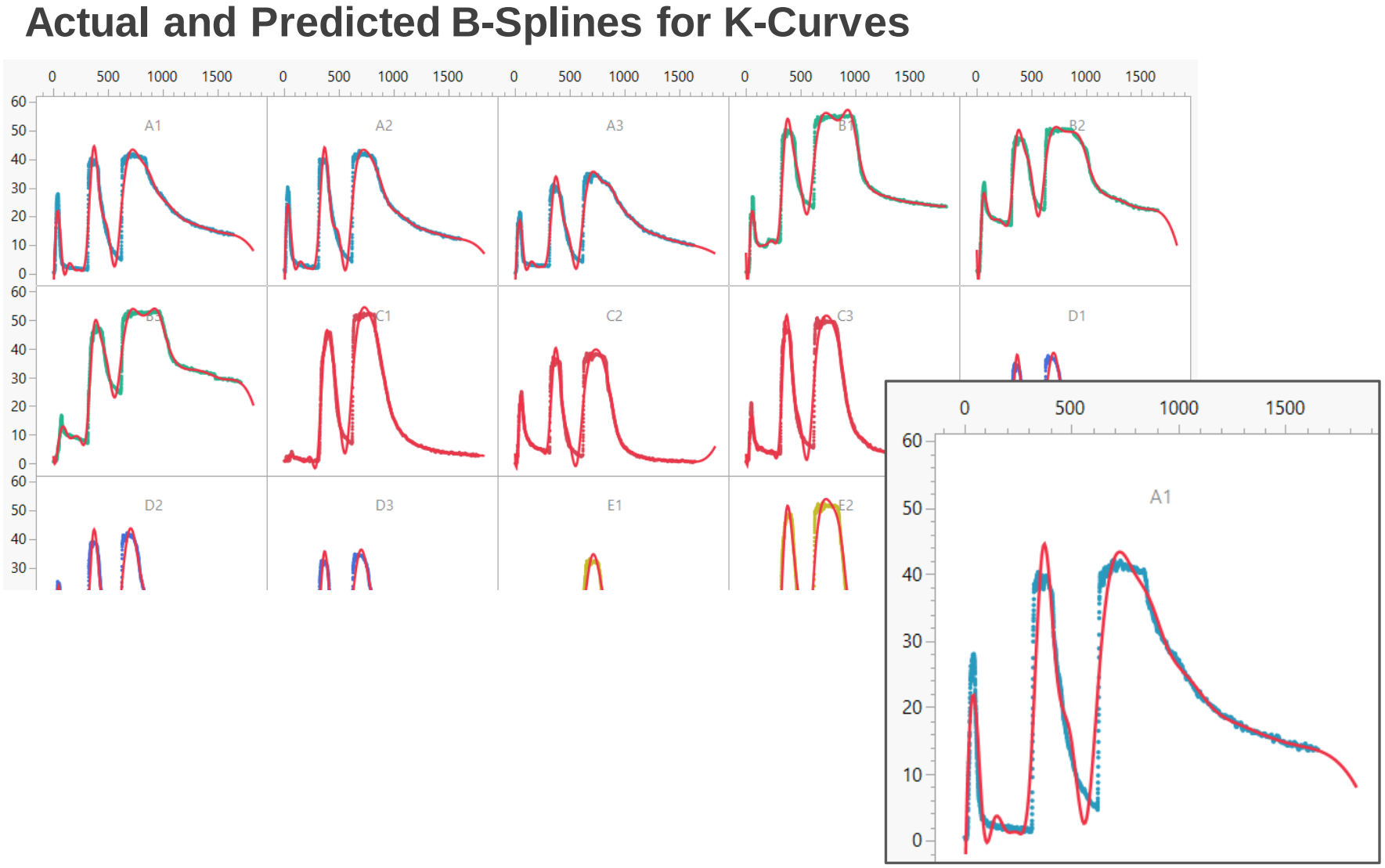
How to analyze K-data curves with JMP Functional Data Explorer (FDE)

- Note: JMP 16 Early Adopter 8 used for demo

FDA Findings

Curve fitting:

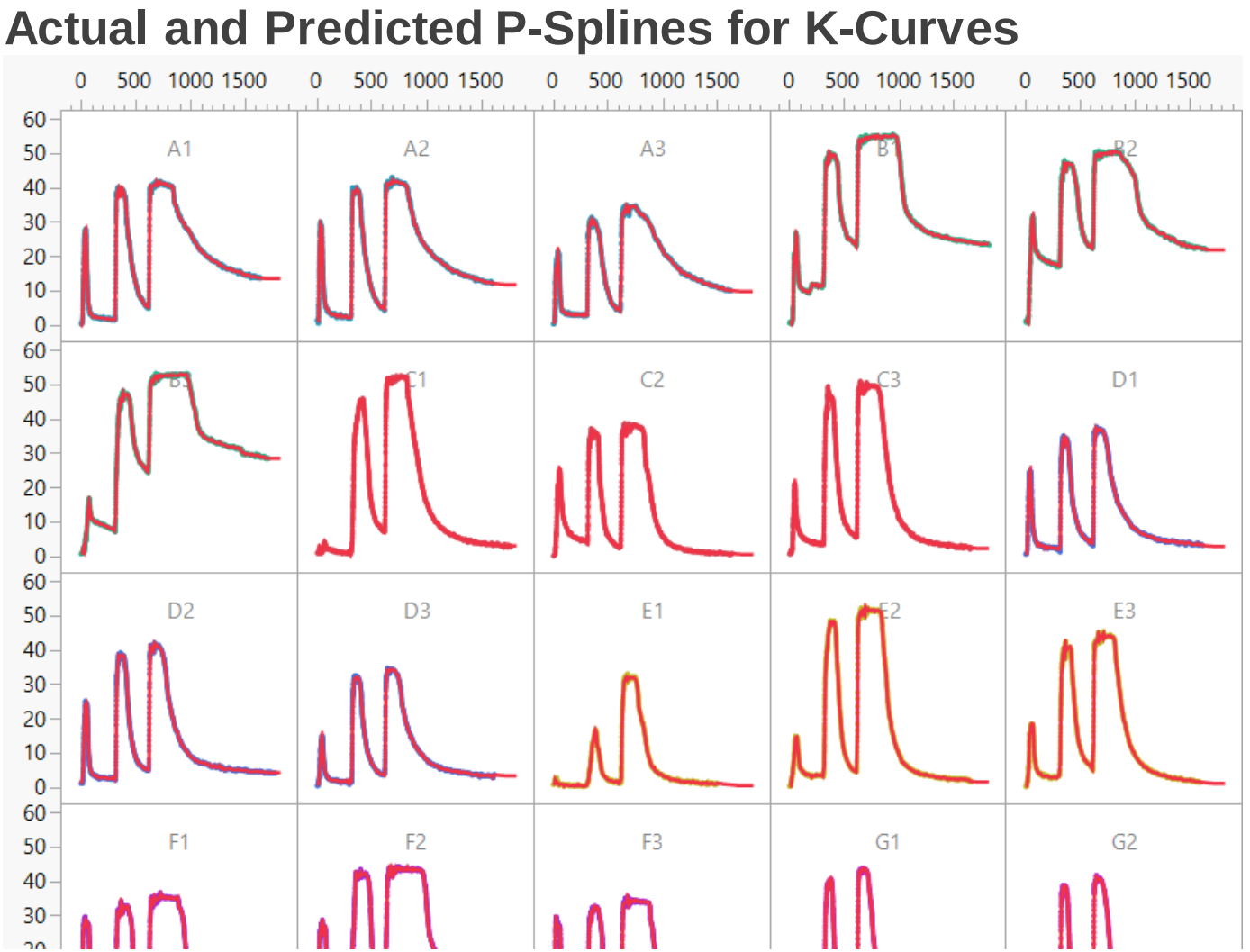
- Red line is fit, any other colour is measurement data
- B-Splines not accurately dealing with step changes in discrete measures.



FDA Findings

Curve fitting:

- P-Splines Step-function much better suited.
- P-Splines fits of smoothened K-curves look really good

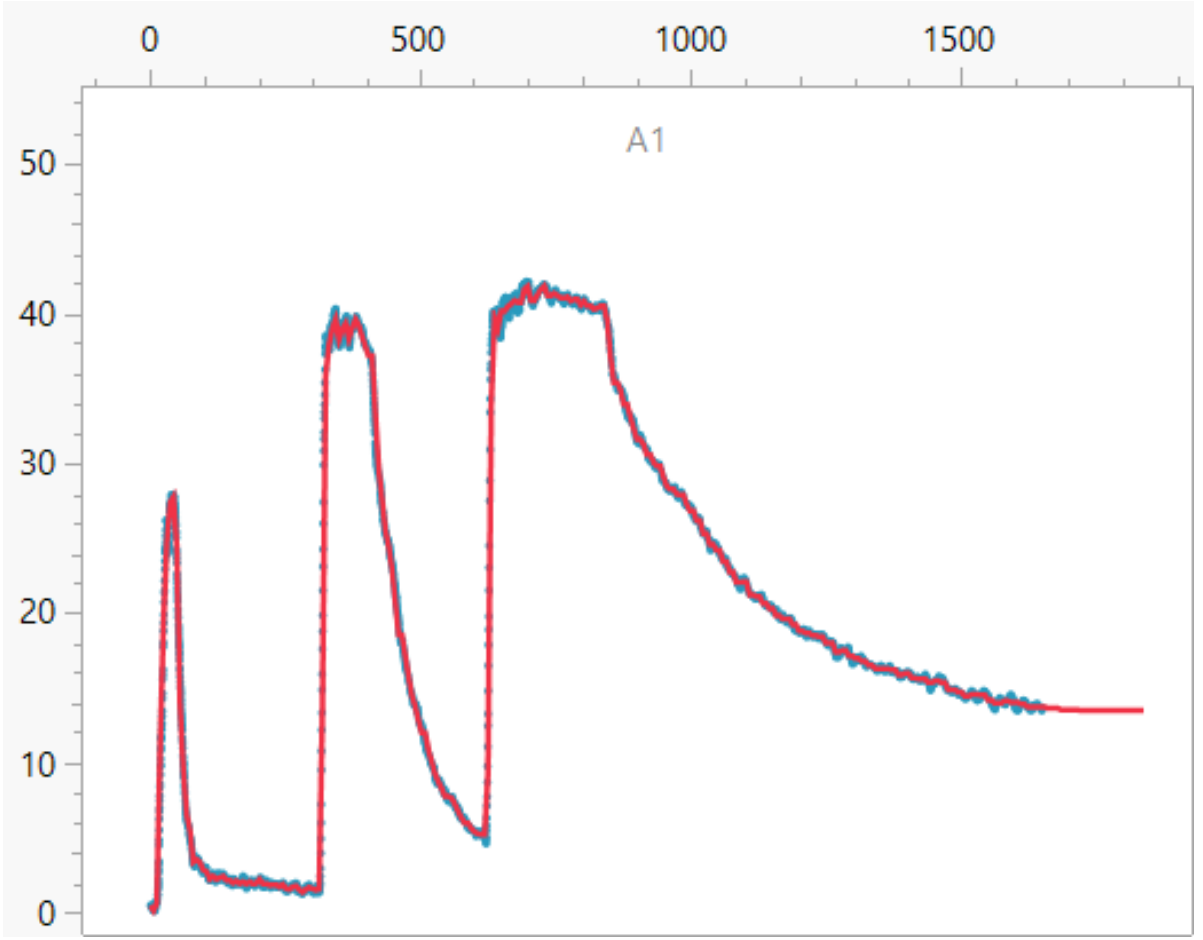


FDA Findings

Curve fitting:

- P-Splines step function still captures some measurement noise.

Actual and Predicted P-Splines for Kinetics-Curves

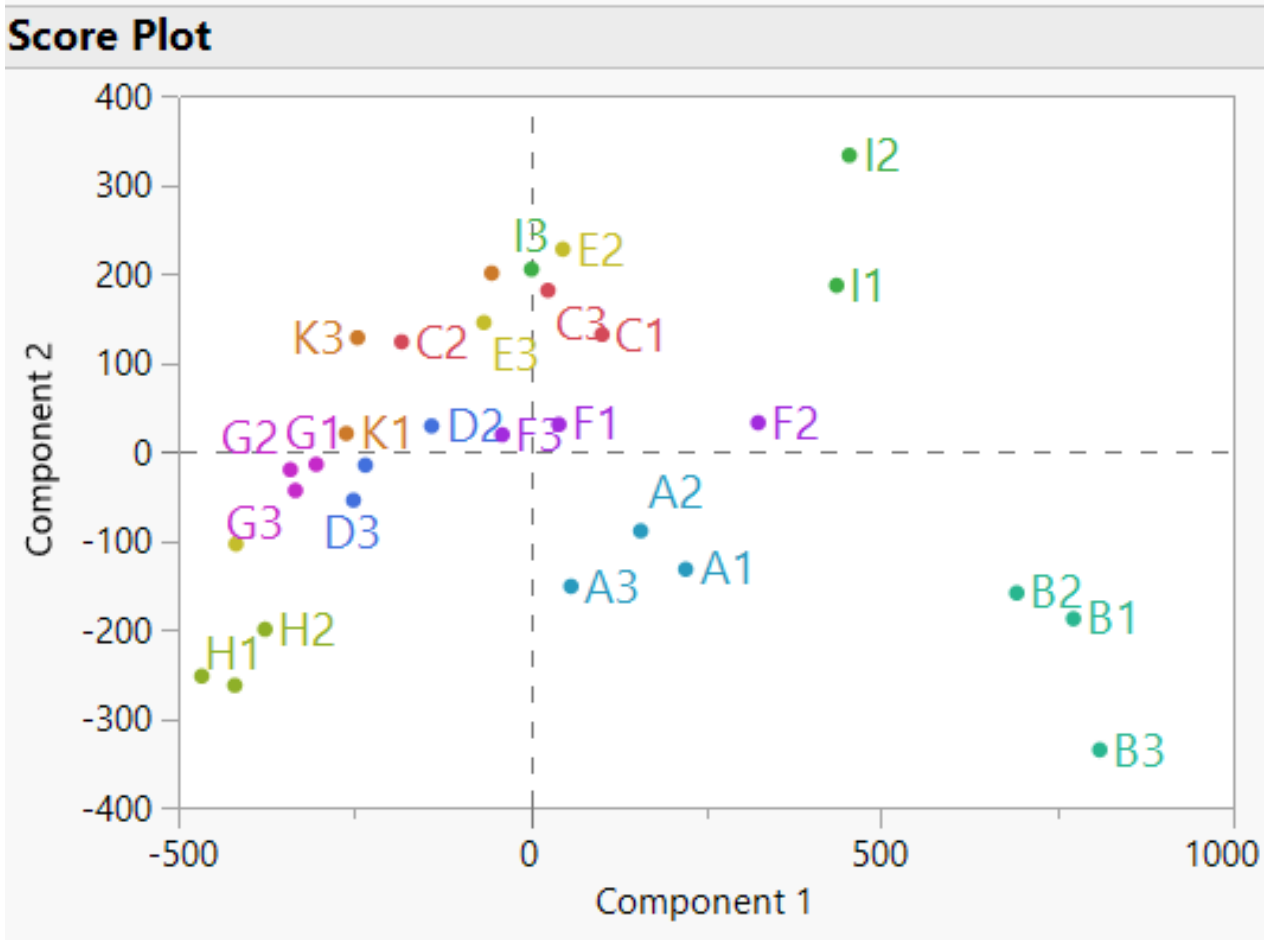


FDA Findings

Calculate Functional Principal Components (FPC) from Curve fit

Plot first 2 FPCs:

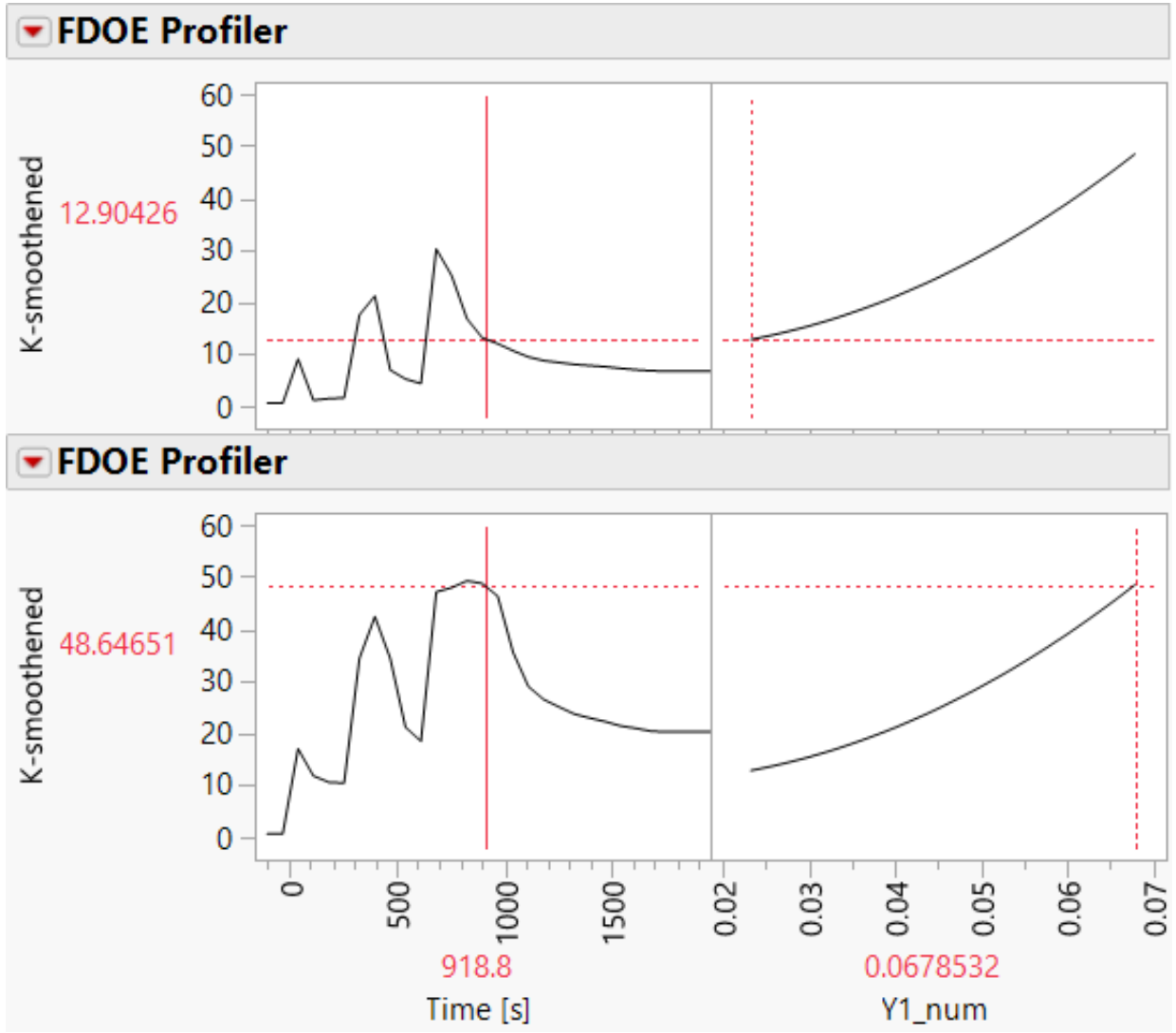
- Can see some product differences. Product replicates often group together; some not
- Most of the variability seen is coming from products



FDA Findings

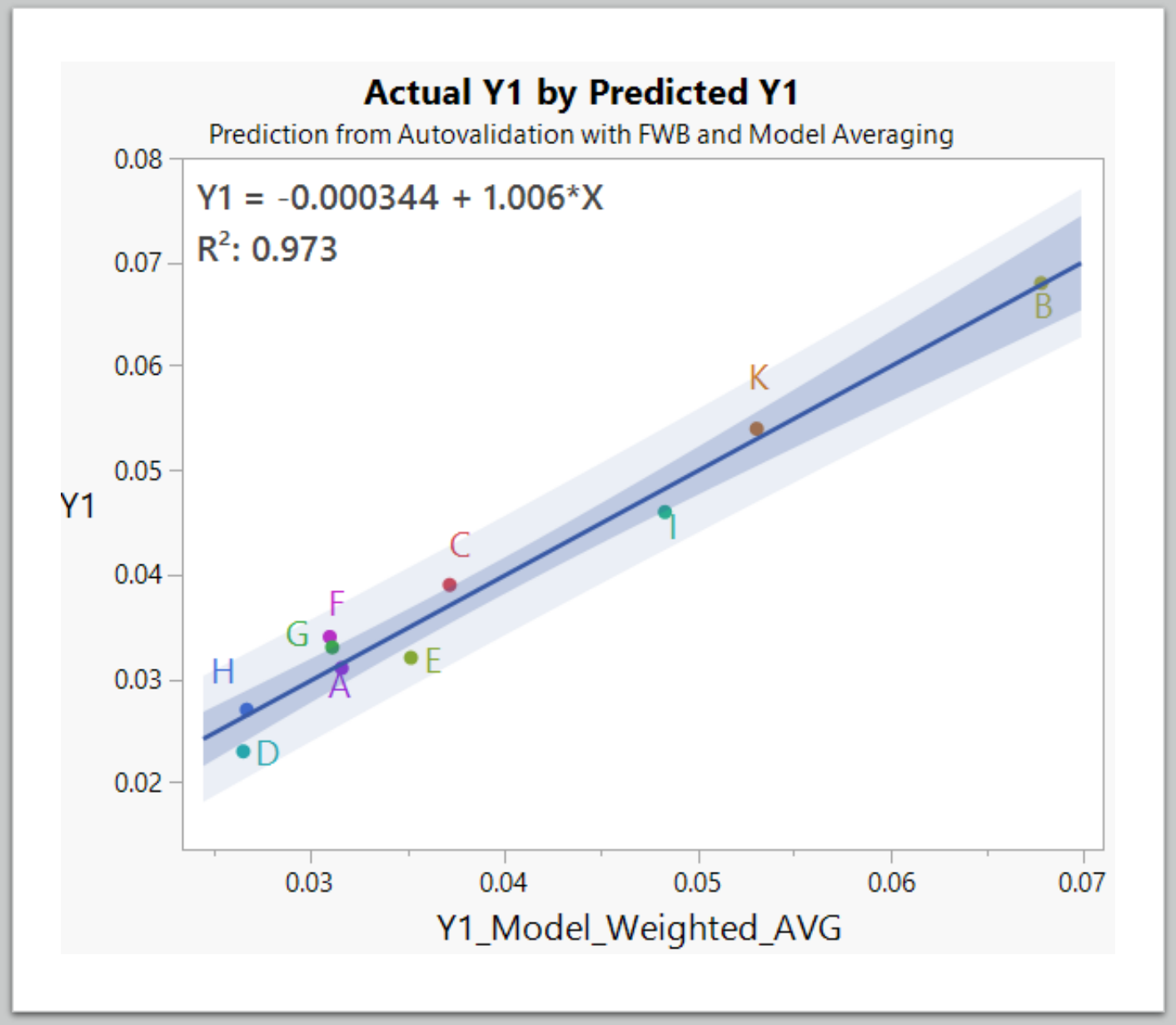
Functional DOE Profiler:

- The real purpose of JMP's FDE: Use the DOE capability of JMP
- Plotting K-curve predictions against Yield 1 performance
- Identify how good (top) Y1 curve compares to bad (bottom) Y1 curve
- Can do that for each Response of interest to visually understand what curves drive which consumer perception



JMP Y1 Predictions

- Use FDA *Function Summaries* with Auto-Validation, Weighing, and Model Averaging (*)
- R-Square = 0.97
- Press R-Square: 0.90
- Too good to be true?!!



(*) reference to auto-validation and model averaging (JMP Community)

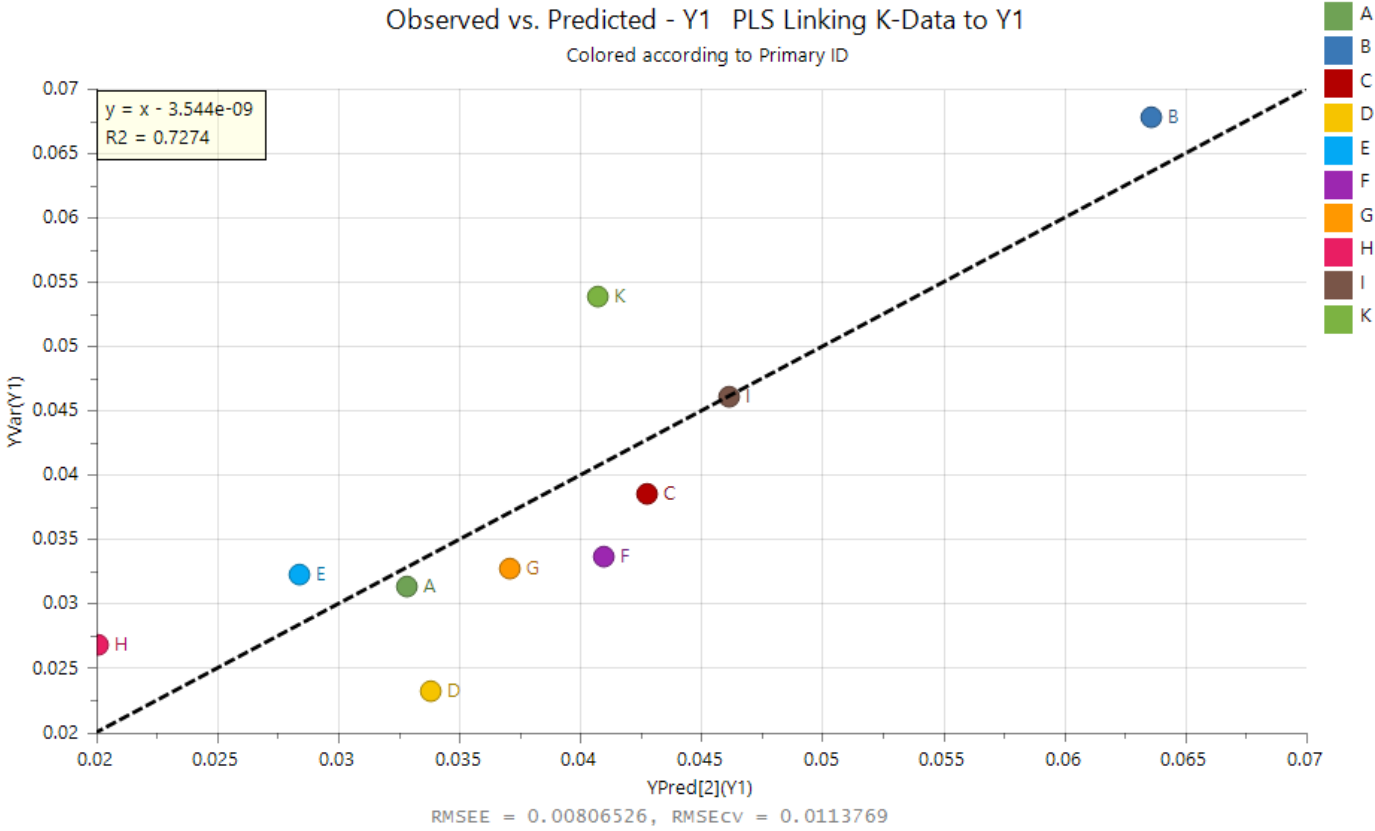
PLS - Predicting outcomes

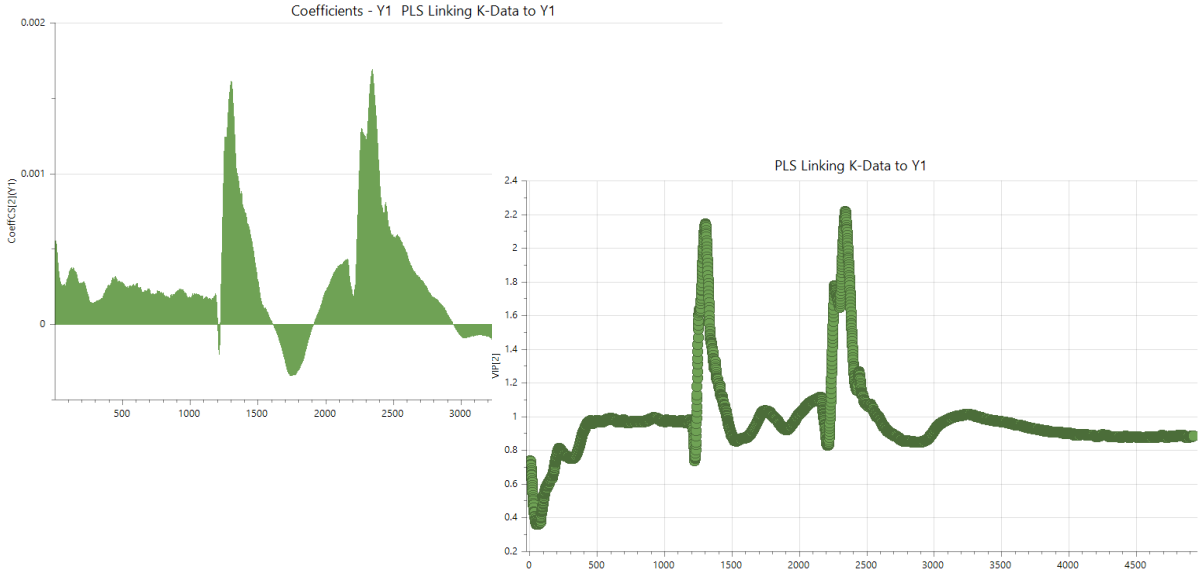
Looks like an OK(ish) model:

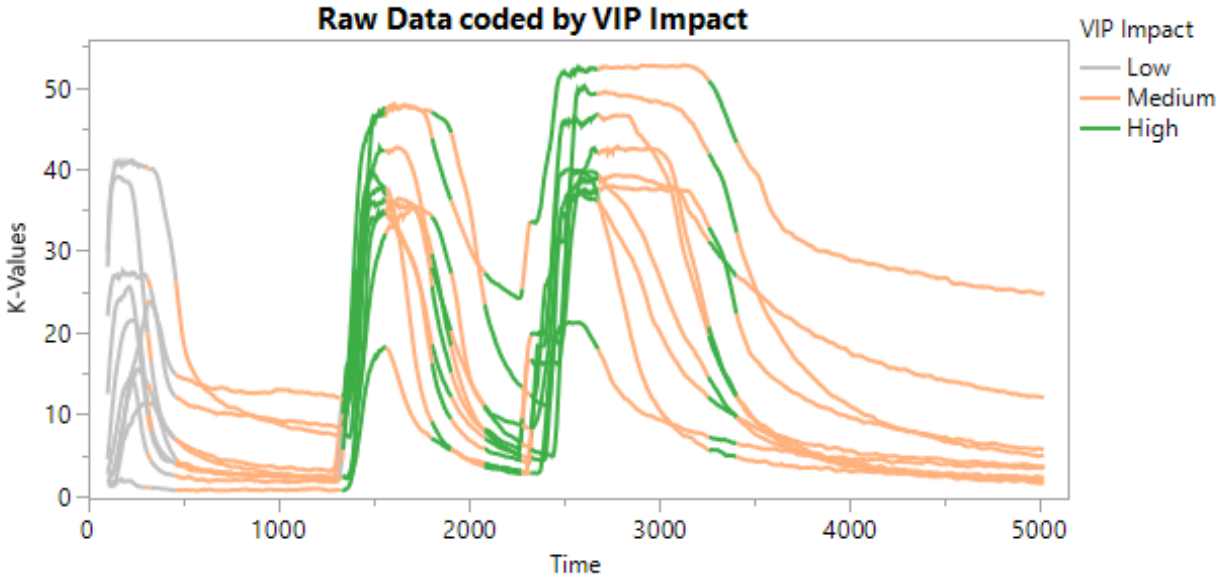
- R^2 is 73% and fit looks suitable
- Maybe an influence from B?

Cross-Validation measures (Q^2) are quite low at only 33%.

However, can get some idea of the regions that impacts predictions.







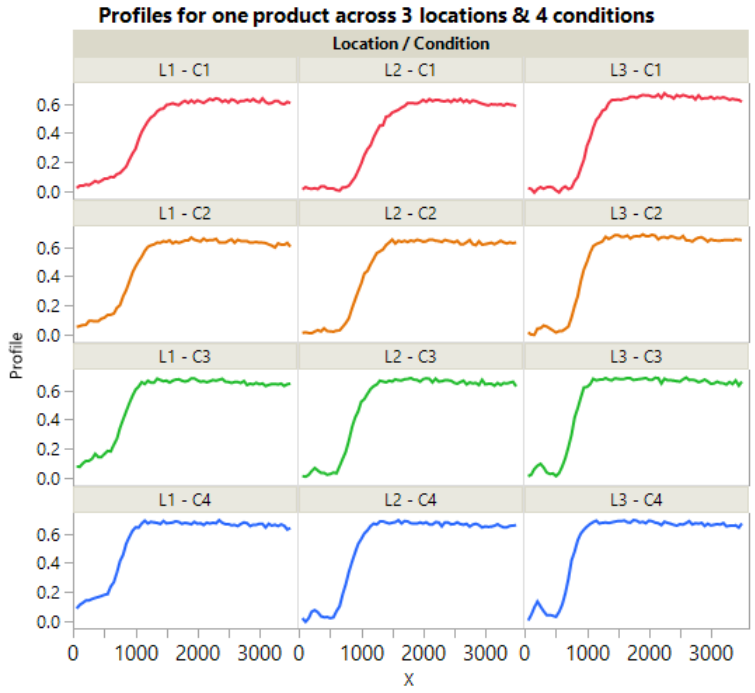
P-Data Curves – Multiple Traces

When assessing curves, we look at 4 conditions at three locations

- Conditions: C1 – C4
- Locations: 1 - 3.

We also have measures taken at C5 at location 1 only

- Different curve obtained as on a different device.



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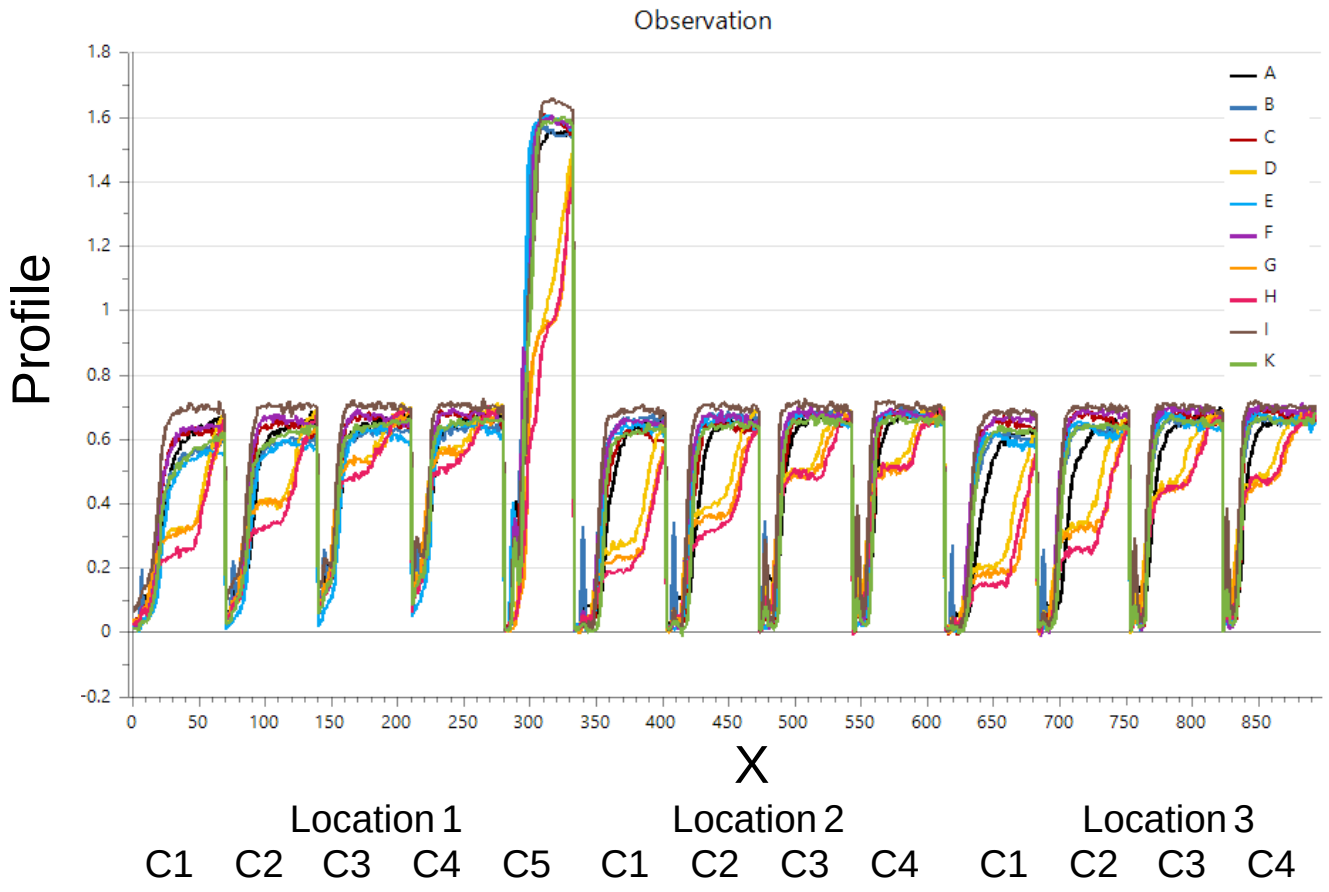
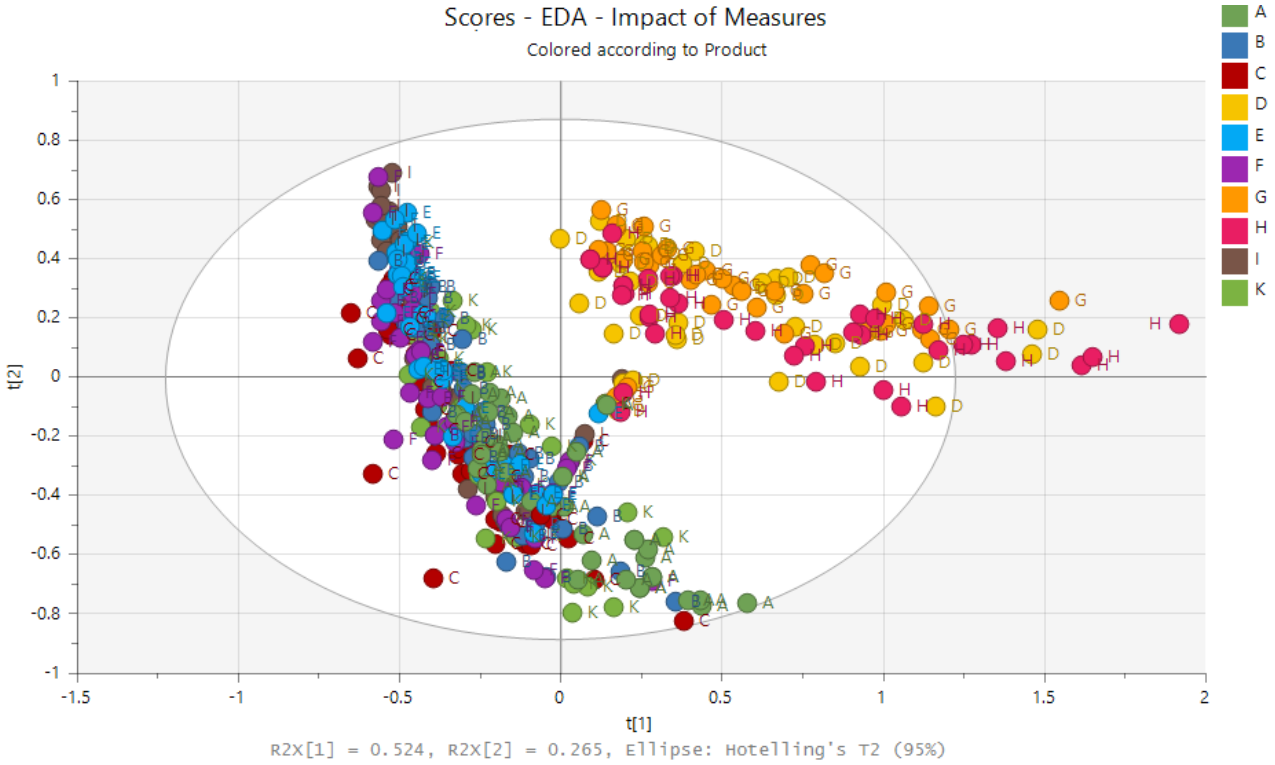
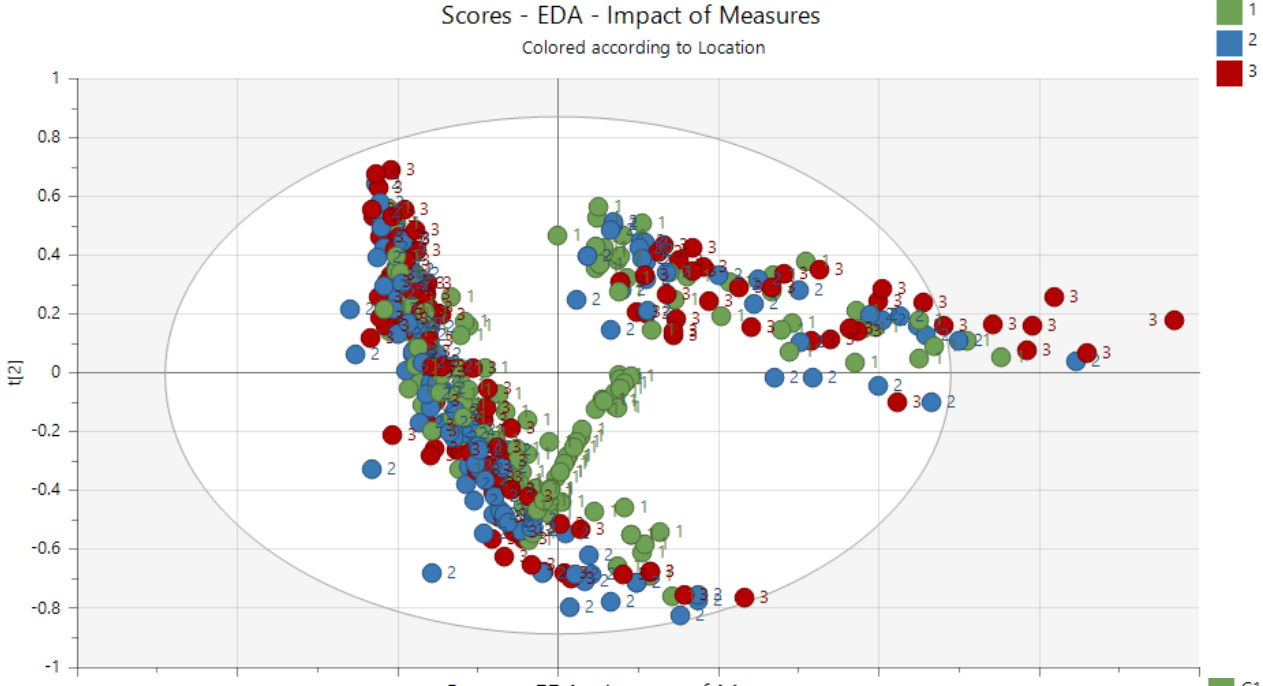
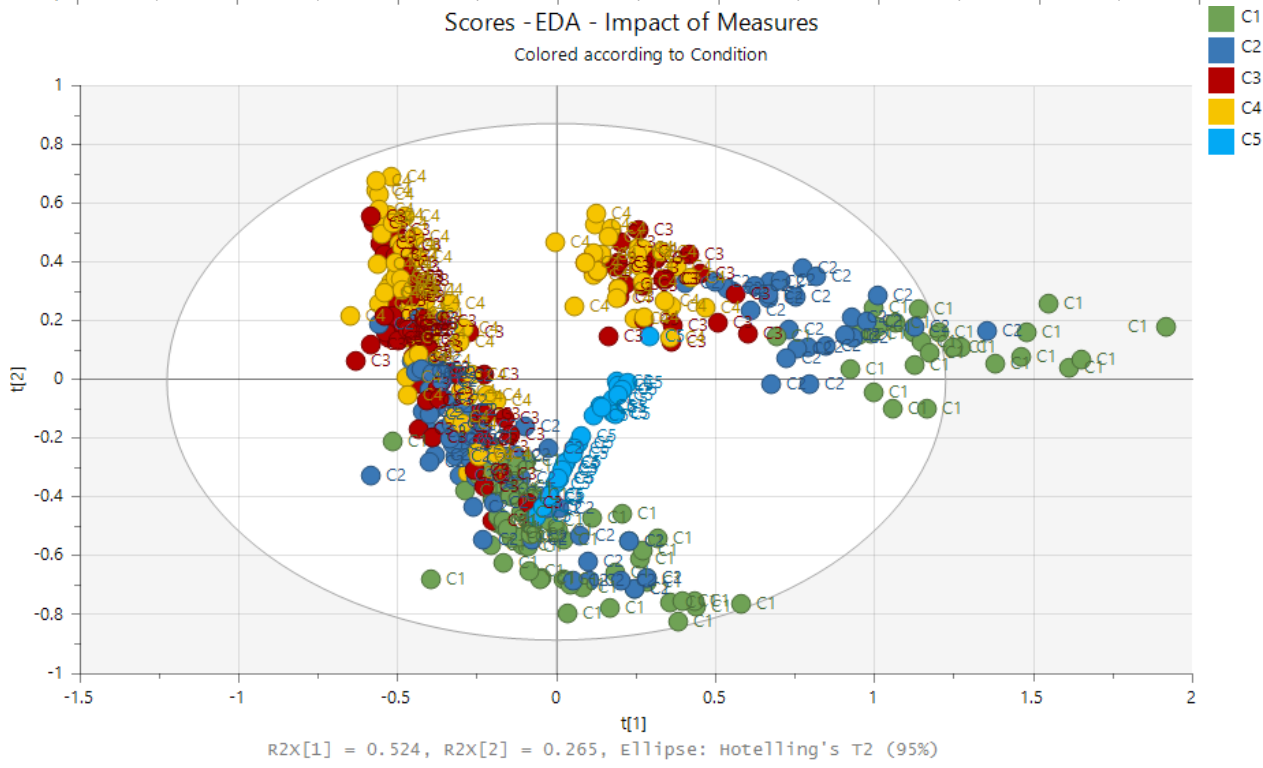


P-Data Curves – PCA





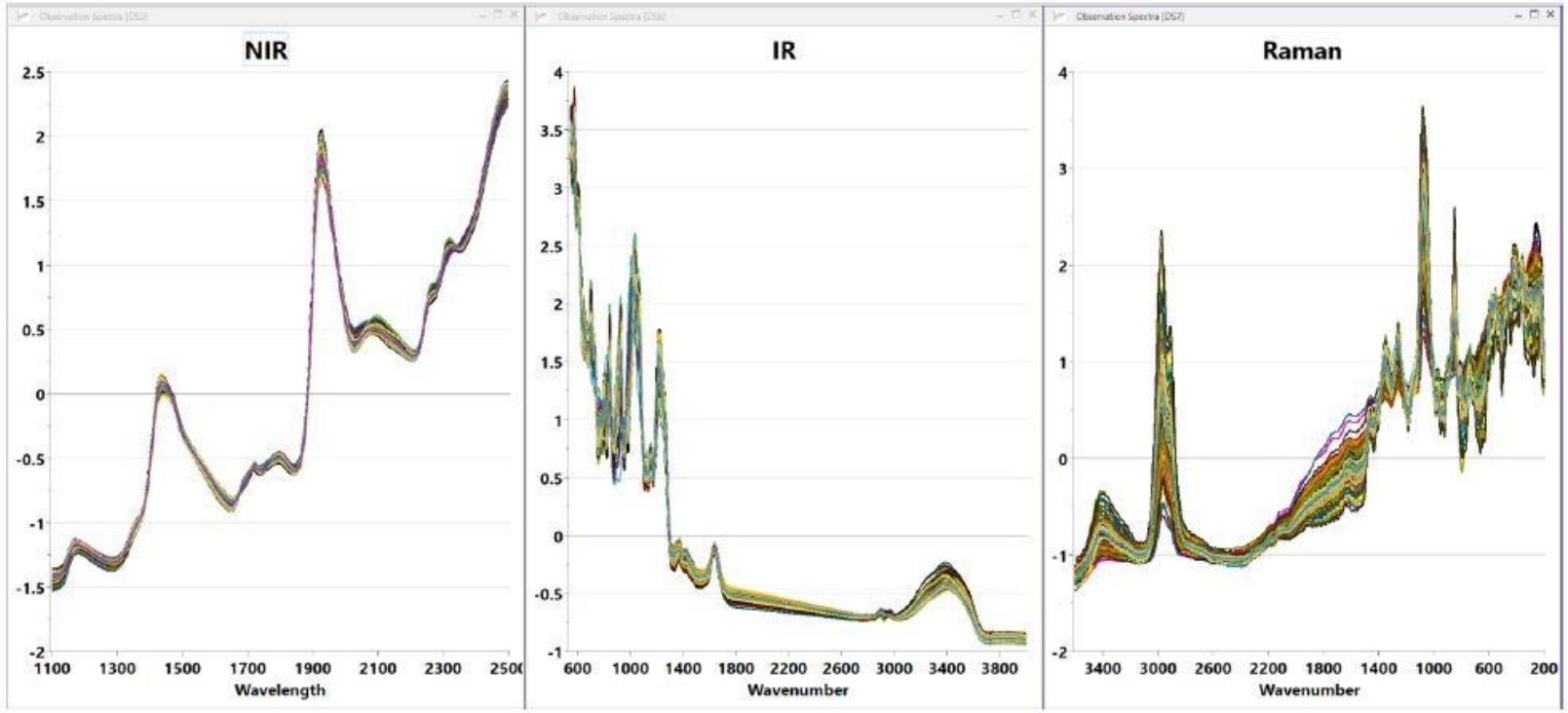


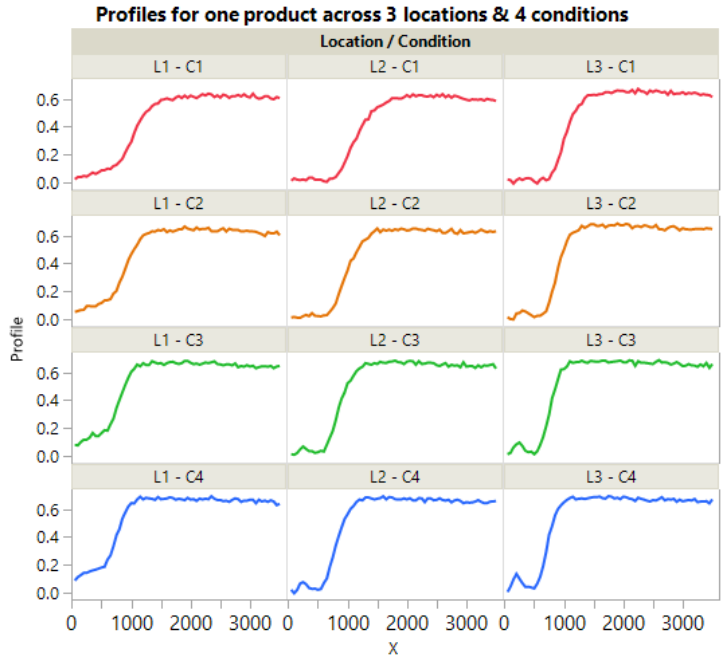
- Clear to differentiate the products into two groups/clusters – they make sense;-)
- No real patterns when colour by location
- Can see patterns due to the condition applied during measurement.

We shall focus on the location = 3 for now.

Multiblock Orthogonal Component Analysis (MOCA) & Hierarchical Modelling

- Can look at ‘blocks’ of data - normally different spectra.
  - Assess links between blocks – if they are not unique, potential redundancy.
  - Assess impact of each block on a response.





For our data – do we see overlap between the different locations and conditions?

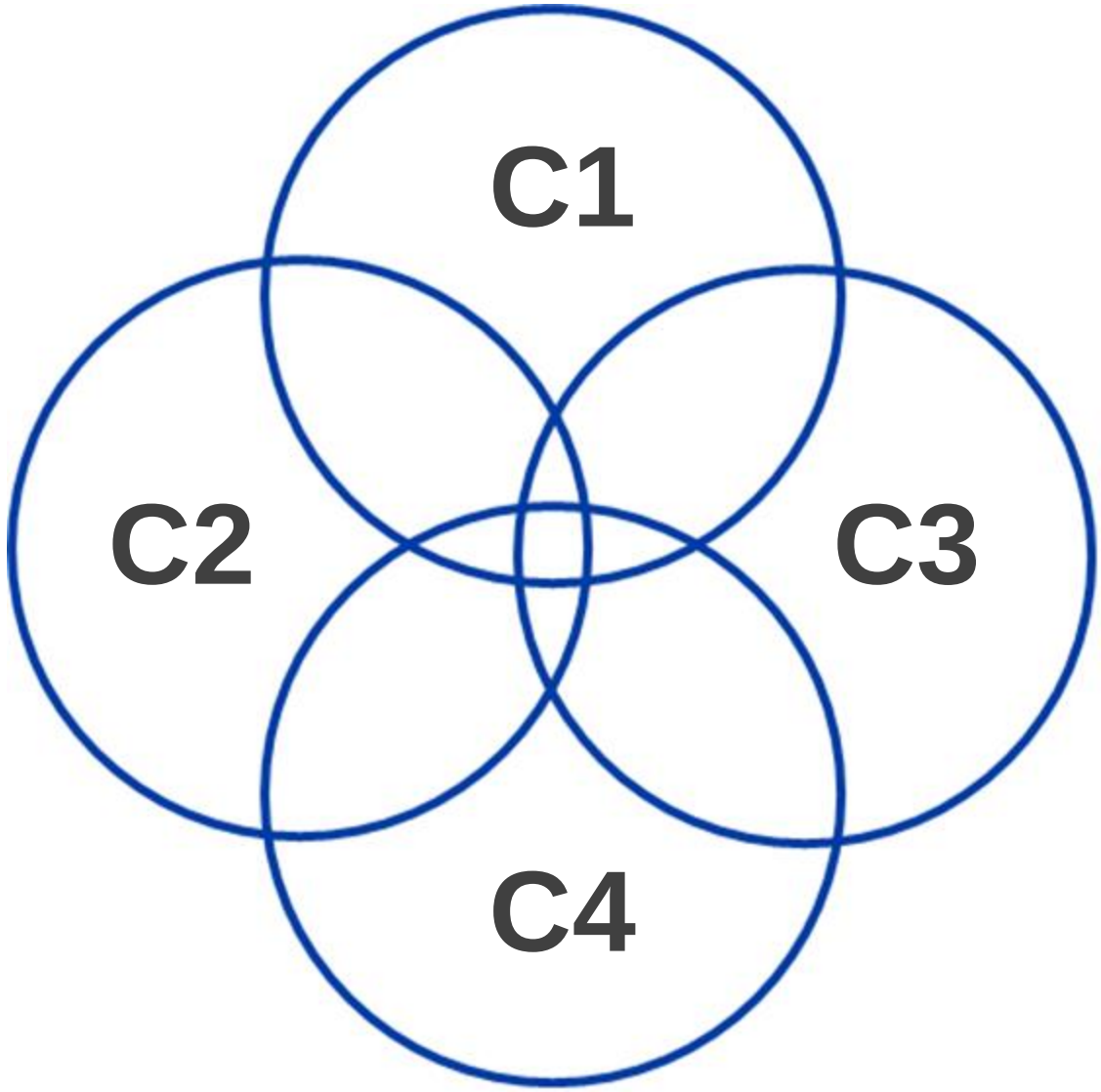
Multiblock Orthogonal Component Analysis
MOCA

Consider the four conditions at location **3**, and how the data may overlap.

The figure shows the case where we see some overlap between conditions.

We can see three forms of ‘overlap’

- **Globally Joint information**
- **Locally Joint information**
- **Unique information**



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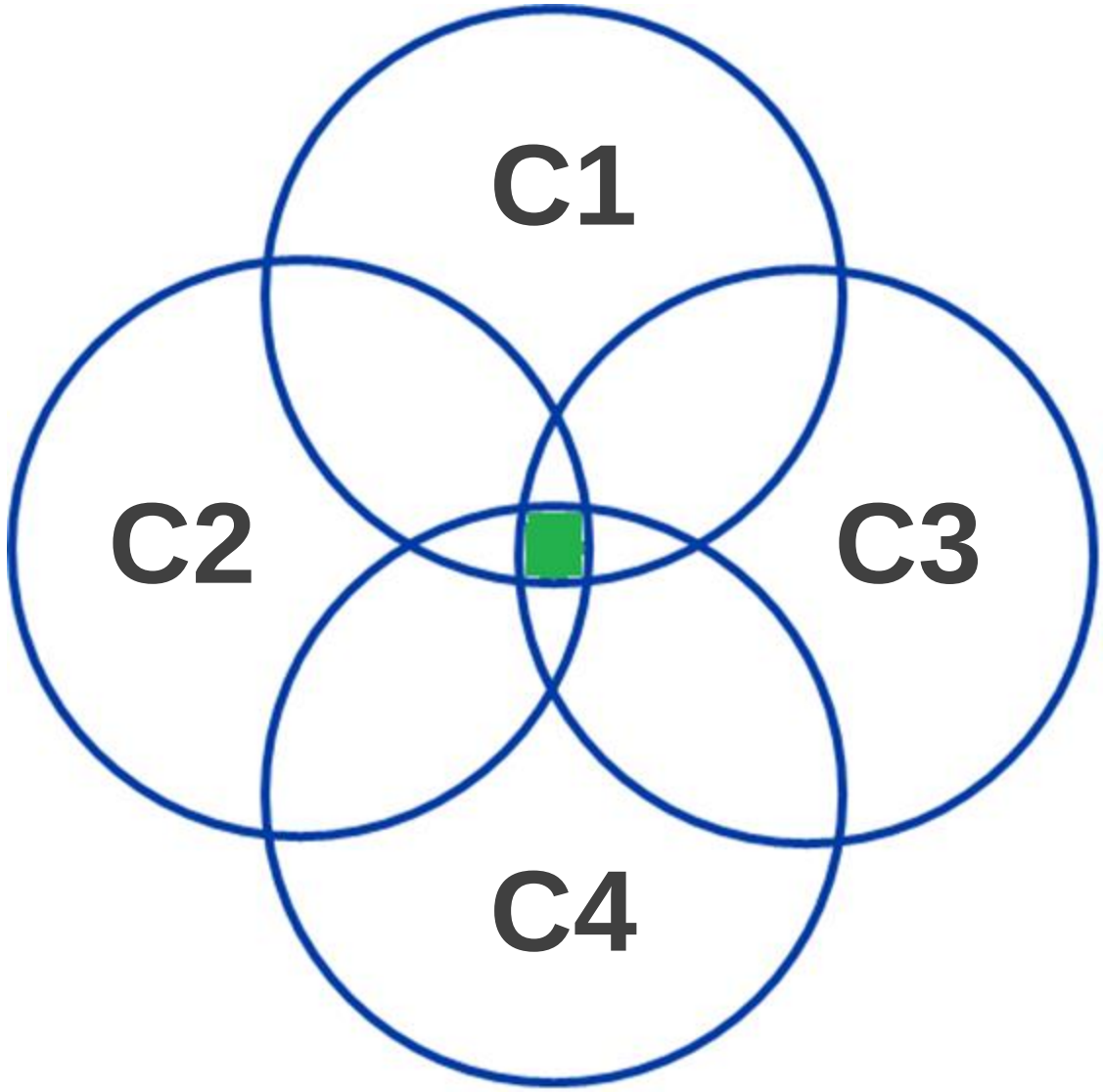

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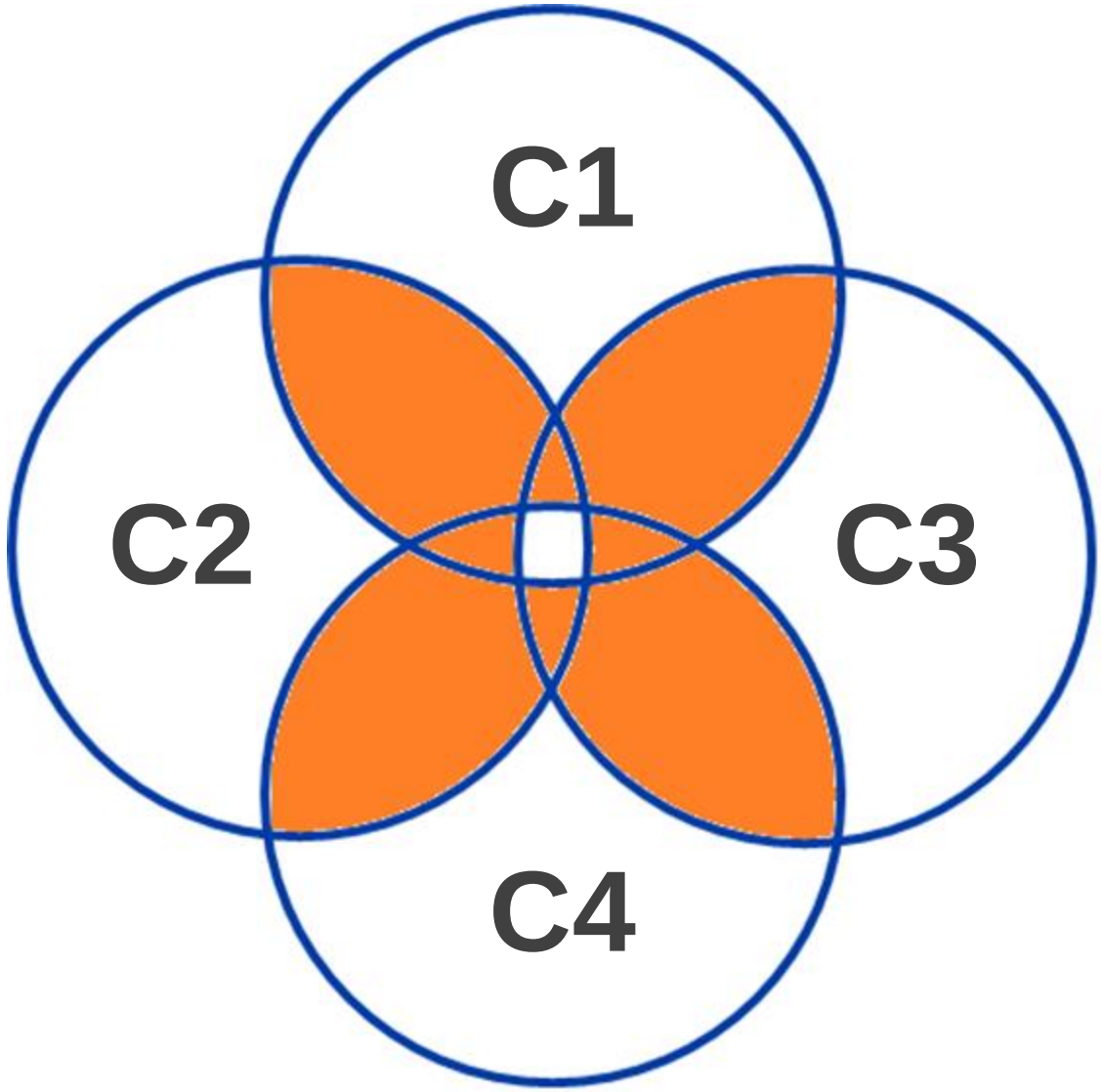

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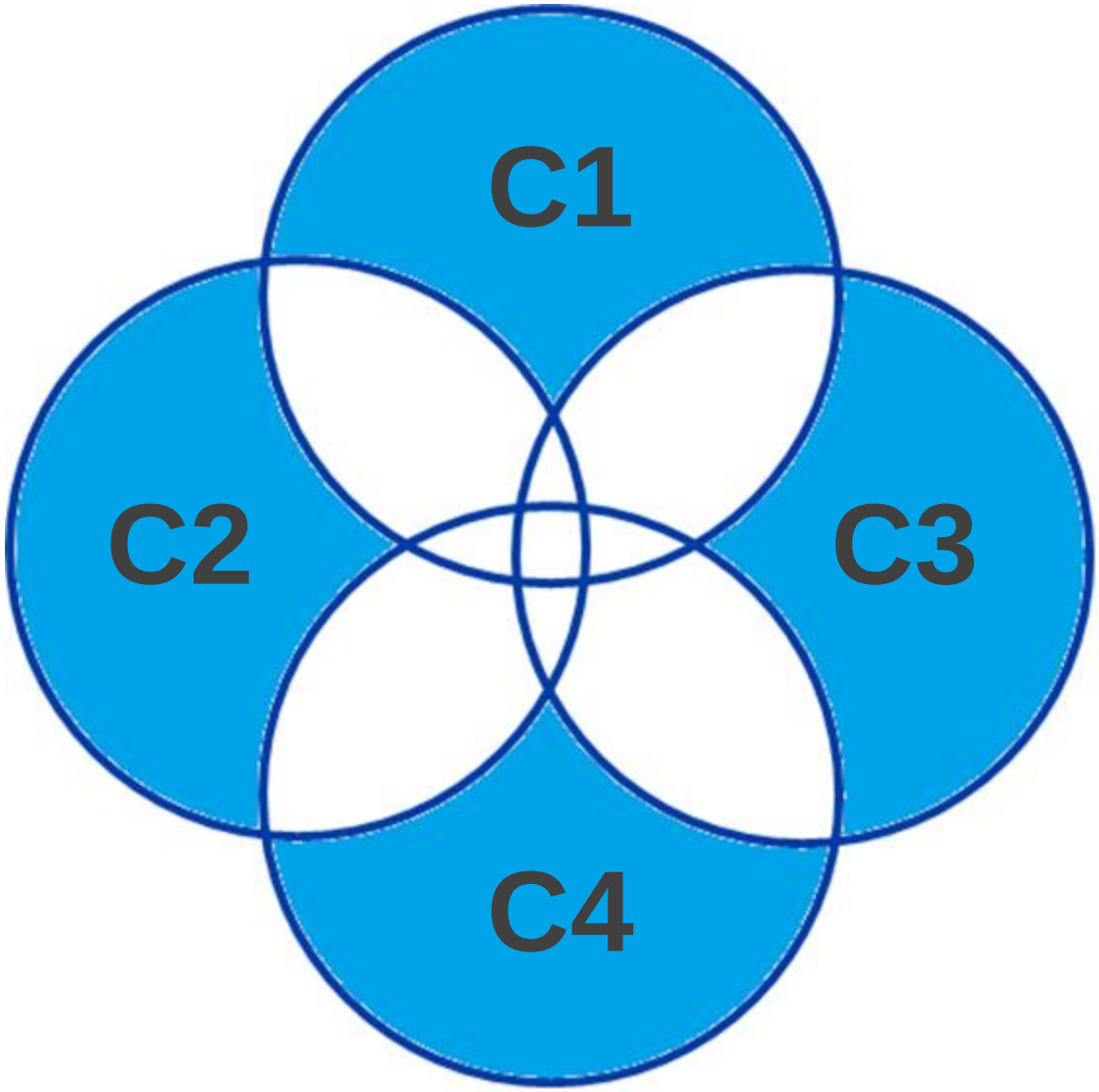

Multiblock Orthogonal Component Analysis

MOCA

Globally Joint information
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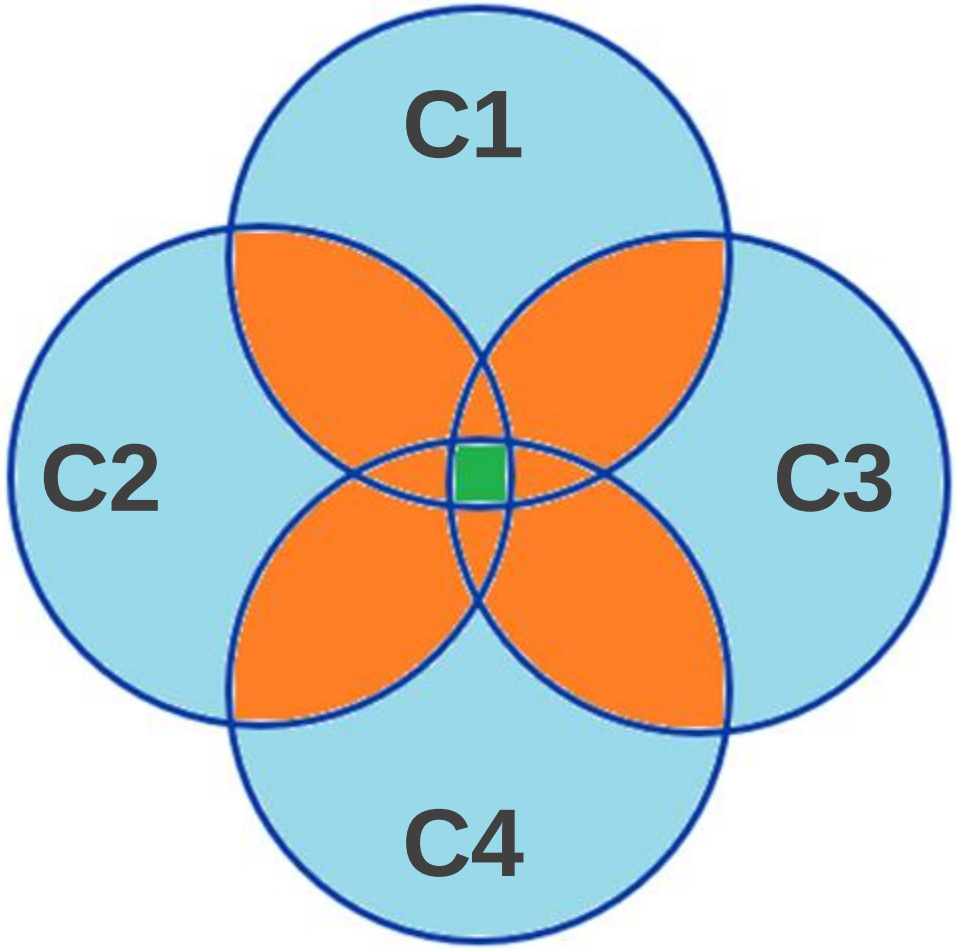
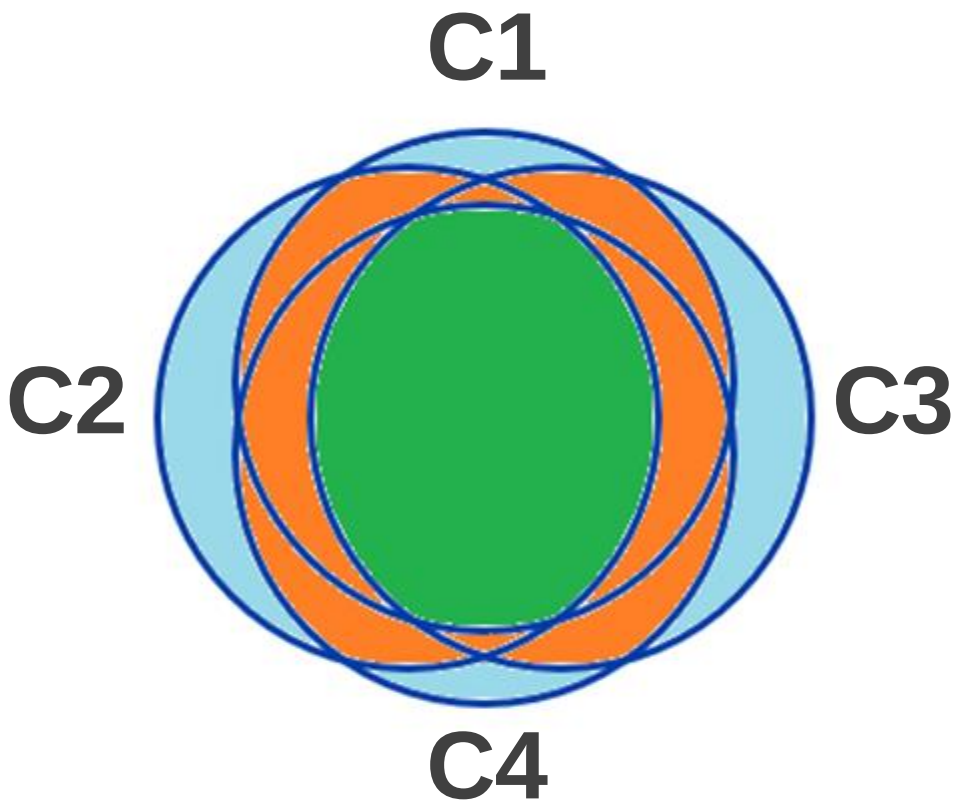


Relatively Unique Information
from each condition



Lots of Joint Information
across conditions

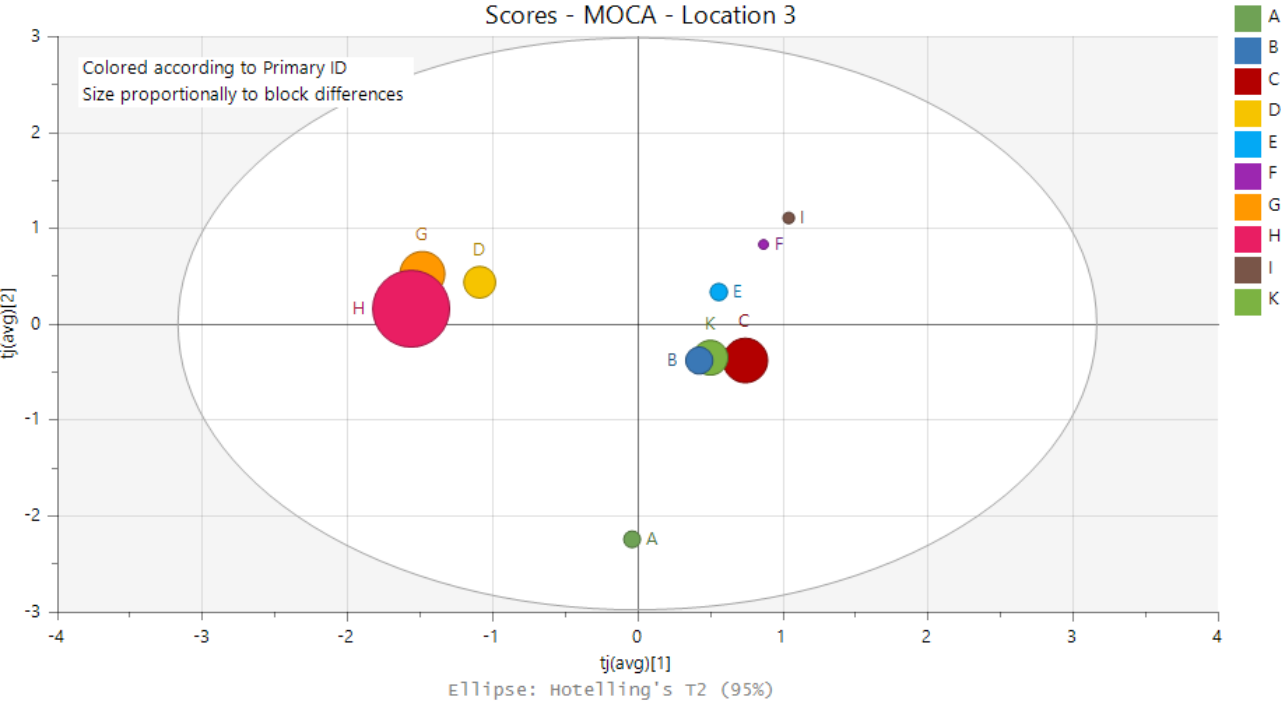
SIMCA MOCA

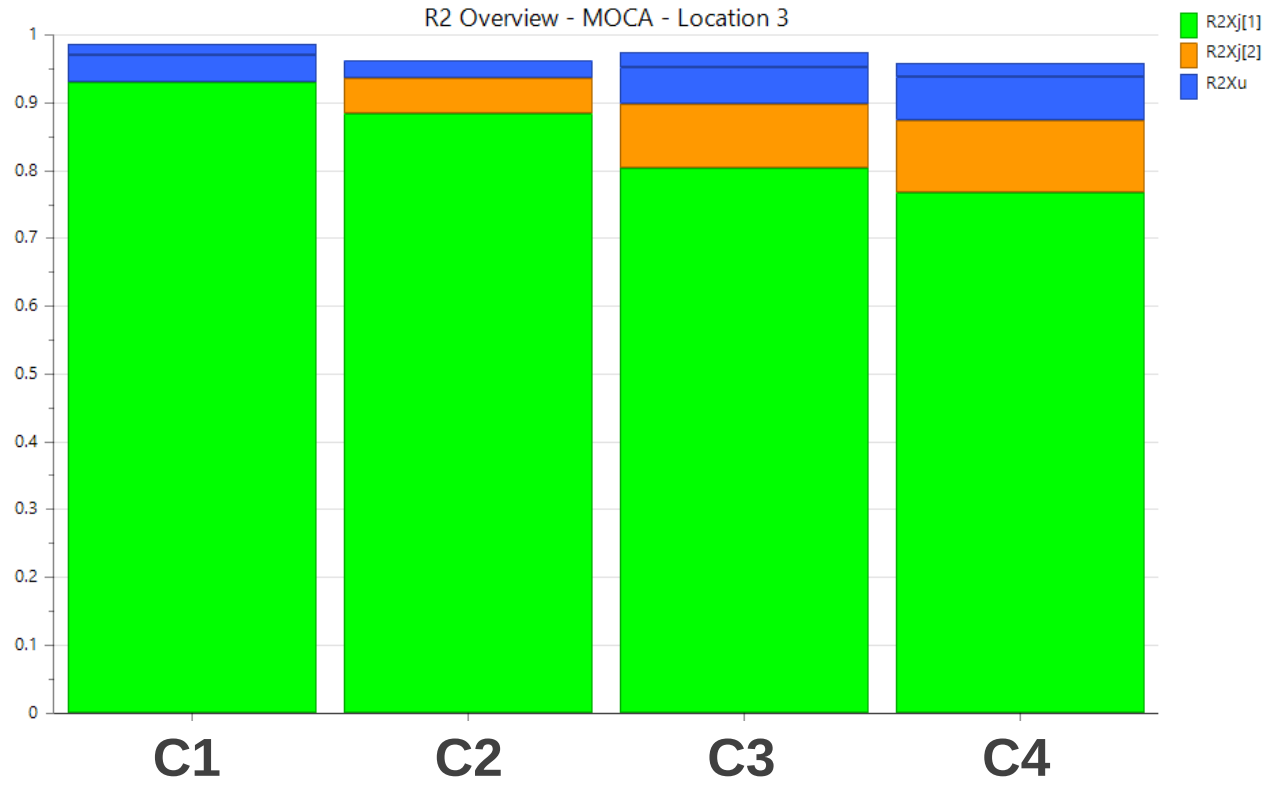
Analysis indicates much overlap between conditions (green & orange) and little uniqueness (blue). Also, product dependent.

Using MOCA & Hierarchal Modelling of Y2:

- C1 @ Locations 1 – 3, and C5 (Location 1)
- $R^2 = 85.5$ & $Q^2 = 69.3$

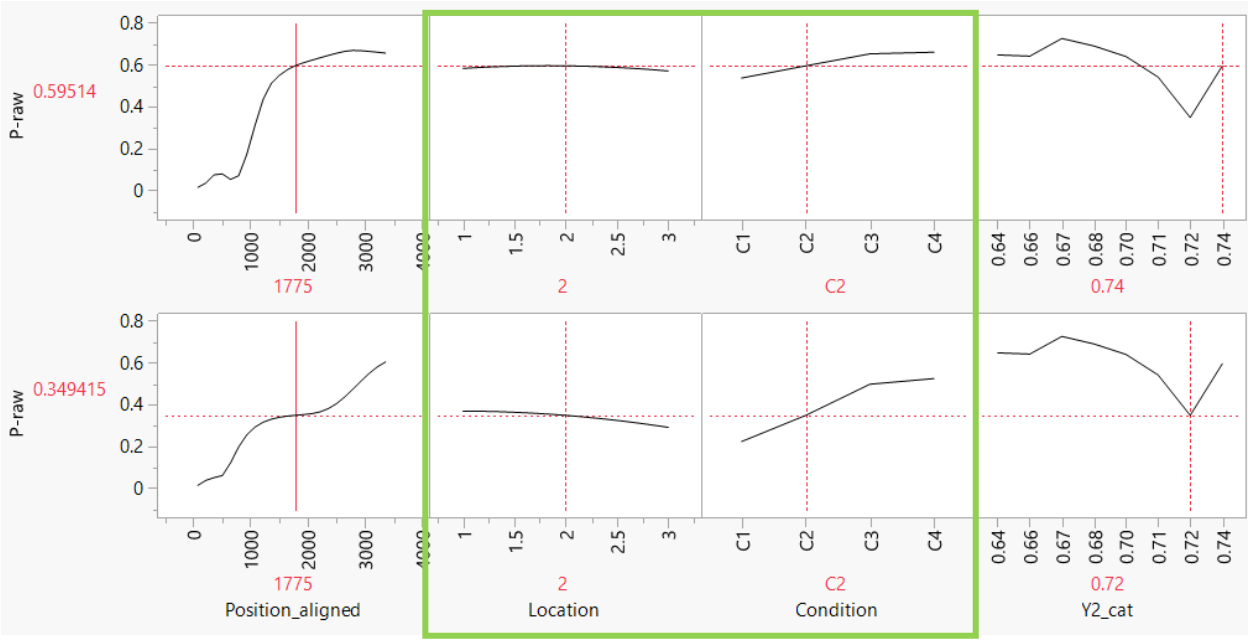
Component	R2X	R2X(cum)	R2X	R2X(cum)	R2X	R2X(cum)	R2X	R2X(cum)
Model		0.987		0.962		0.976		0.959
B	**Location 4**		**C1**		**C2**		**C3**	**C4**
Joint components		0.93		0.937		0.9		0.875
1	0.93	0.93	0.884	0.884	0.805	0.805	0.768	0.768
2	--	--	0.0528	0.937	0.0951	0.9	0.108	0.875
Unique components		0.0565		0.0255		0.076		0.0842
1	0.041	0.041	0.0255	0.0255	0.0524	0.0524	0.0629	0.0629
2	0.0156	0.0565	--	--	0.0236	0.076	0.0213	0.0842





P-data Profiles and Y2: FDA Findings

- Location has less impact on curve shape than condition



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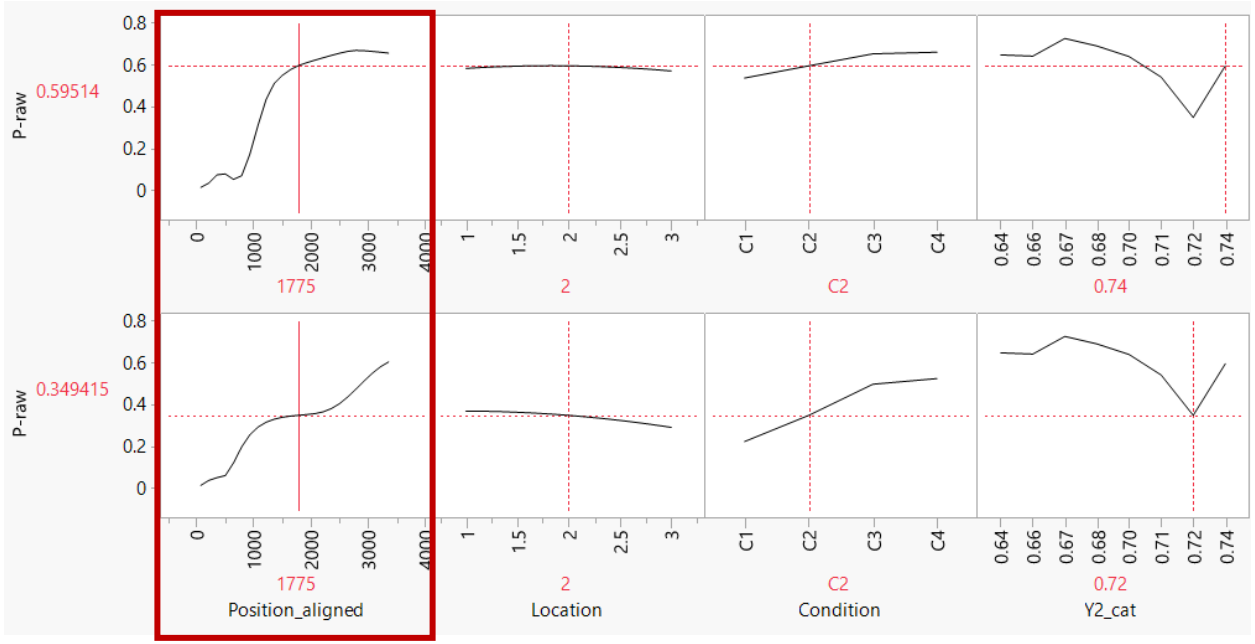
- Curve shapes not “commonly” related to product performance . Is “average curve” = “Golden Curve”? Are there several golden curves?
- Can’t answer yet what location-condition combinations meaningful



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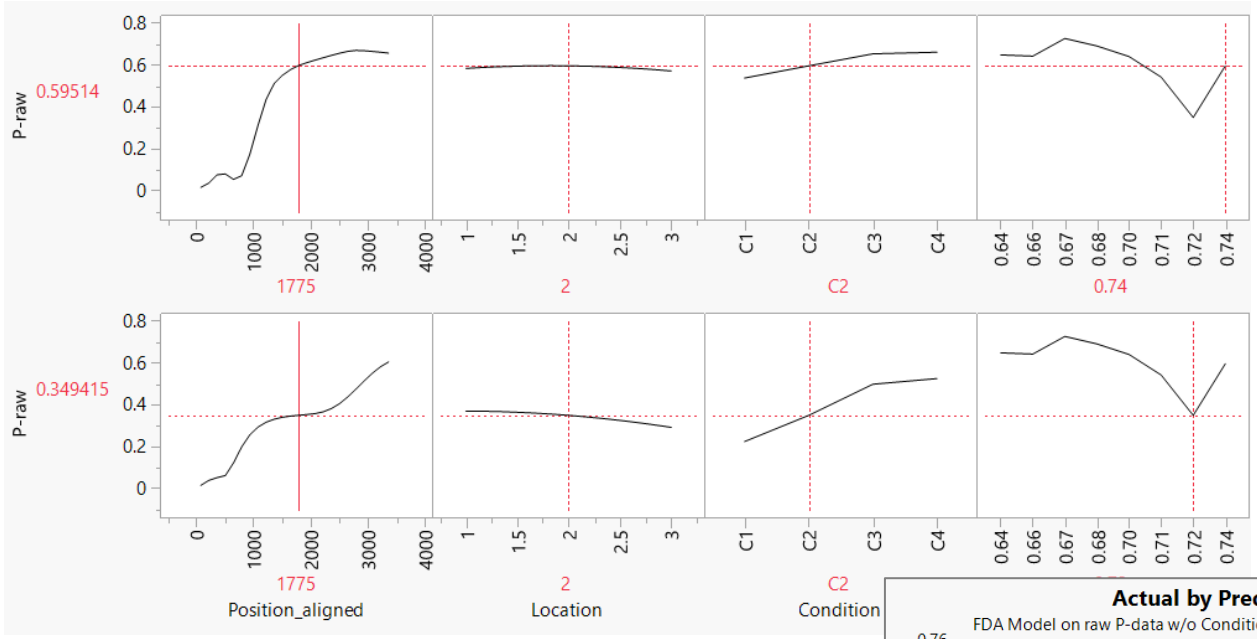
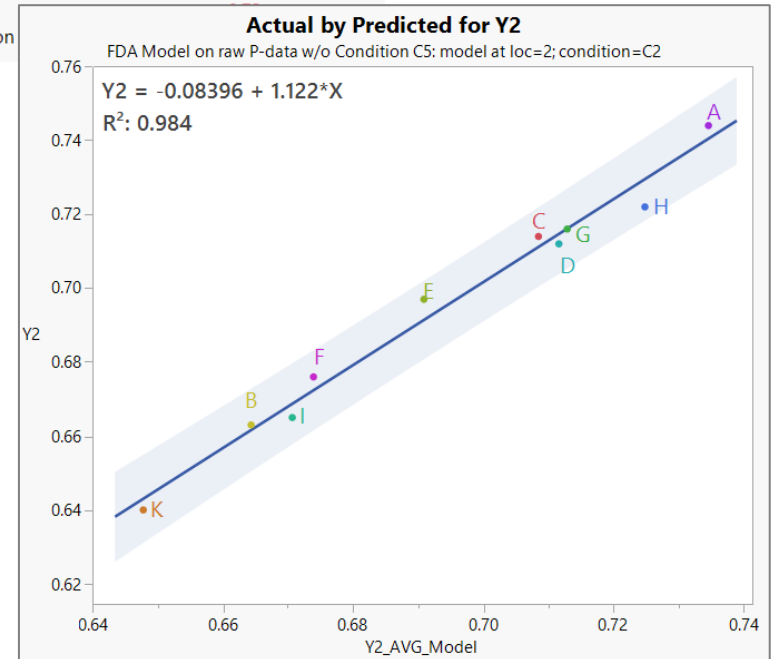
- Can’t answer yet what location-condition combinations meaningful
- Auto-Validation + Model averaging:
  $R^2 = 0.98$
  Press $R^2 = 0.97$





Summary of models

K-Data

FDA:

- Very strong model from FDA
- We can predict curve shape from Yield 1. Do not understand what drives deviations.
- Simple data preparation, but an element of ‚black box‘ modelling.

PLS:

- A relatively strong model (not as good as FDA!).
- Can assess regions of curve that drive Yield 1 – potential for variable selection?
- Not so simple to analyse – element of data prep.

P-Data

PLS:

- MOCA and Hierarchical PLS yield a good model.
- Understanding of regions of curve as well as conditions and locations that drive predictions.

FDA:

- Understanding location and condition impact on curve
- Very good, despite questionable model on Yield 2
- Cannot identify which condition-location combinations needed for Golden Curve understanding.

Summary and Next Steps

Summary

- Simple EDA using FDA and PLS/PCA shows clear patterns, and we can differentiate products.
- With the (limited) data we have, we have a proof of principle to model our Yield responses better than we currently can do.
- The modelling tools have shown which aspects of the data collected drive these predictions and product differentiation.
- Perfect example that ‘too many cooks spoil the broth’ is not always correct – the more tools, the greater the understanding in this case – even if we don't agree.
- Work is ongoing – bugs, new data, feedback, new understandings drive what we are doing.

Next Steps

- External validation of models!!
- More understanding of how different technical measures drive each other – can we simplify what we collect?
- Make use of FDA DoE tools to assess product making and material composition impact on curve shapes.
- Follow-up with JMP on explaining which part/aspect of the curve most impacts Yield predictions. Combine B- and P-Splines?!
- We have nearly caught the ‘golden curve’. However, answers to some of the above will hopefully mean we will eventually capture the curve entirely.

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Thank You

Any Questions?