Getting to Multiway: A Roadmap for Batch Process Data

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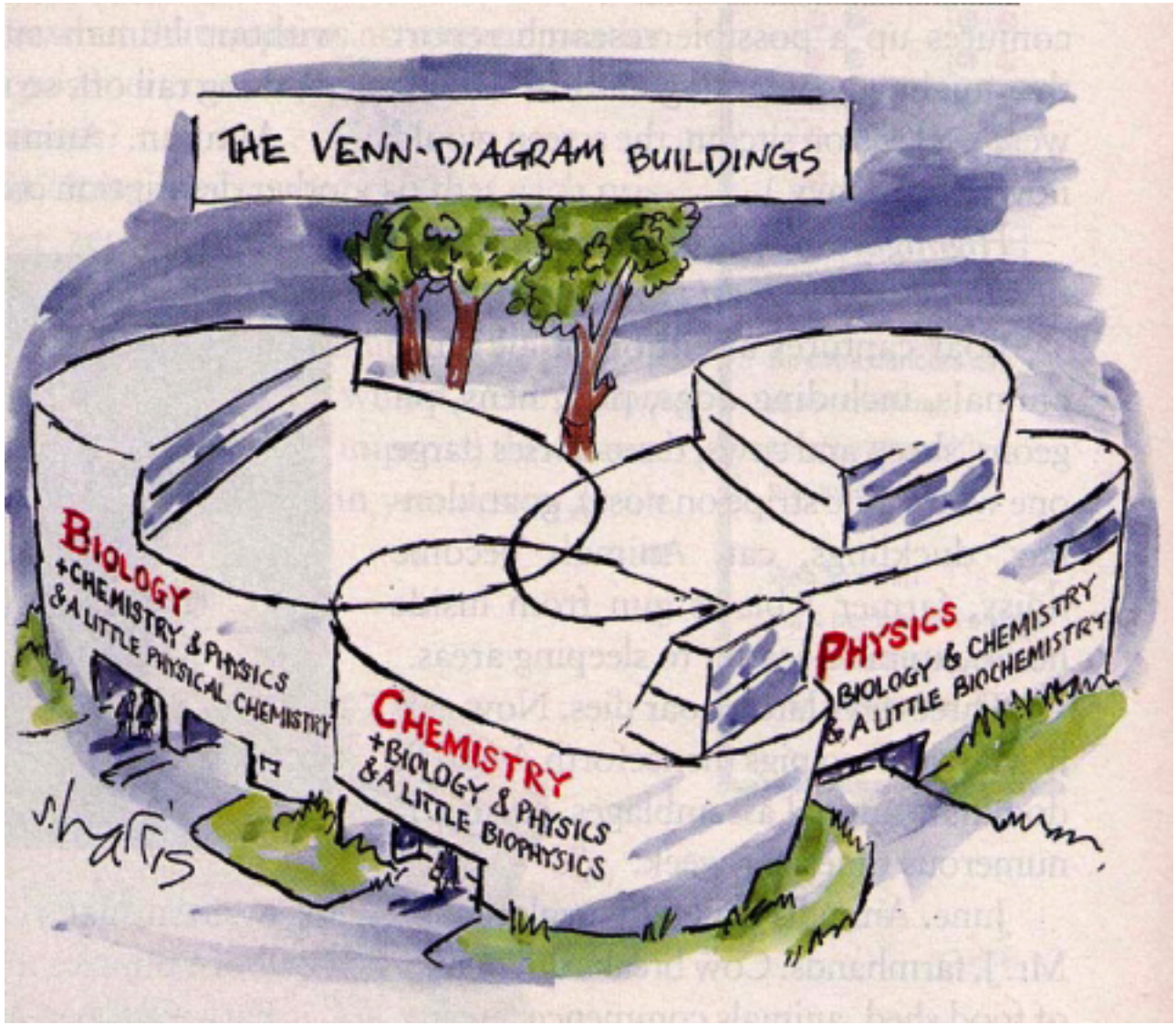

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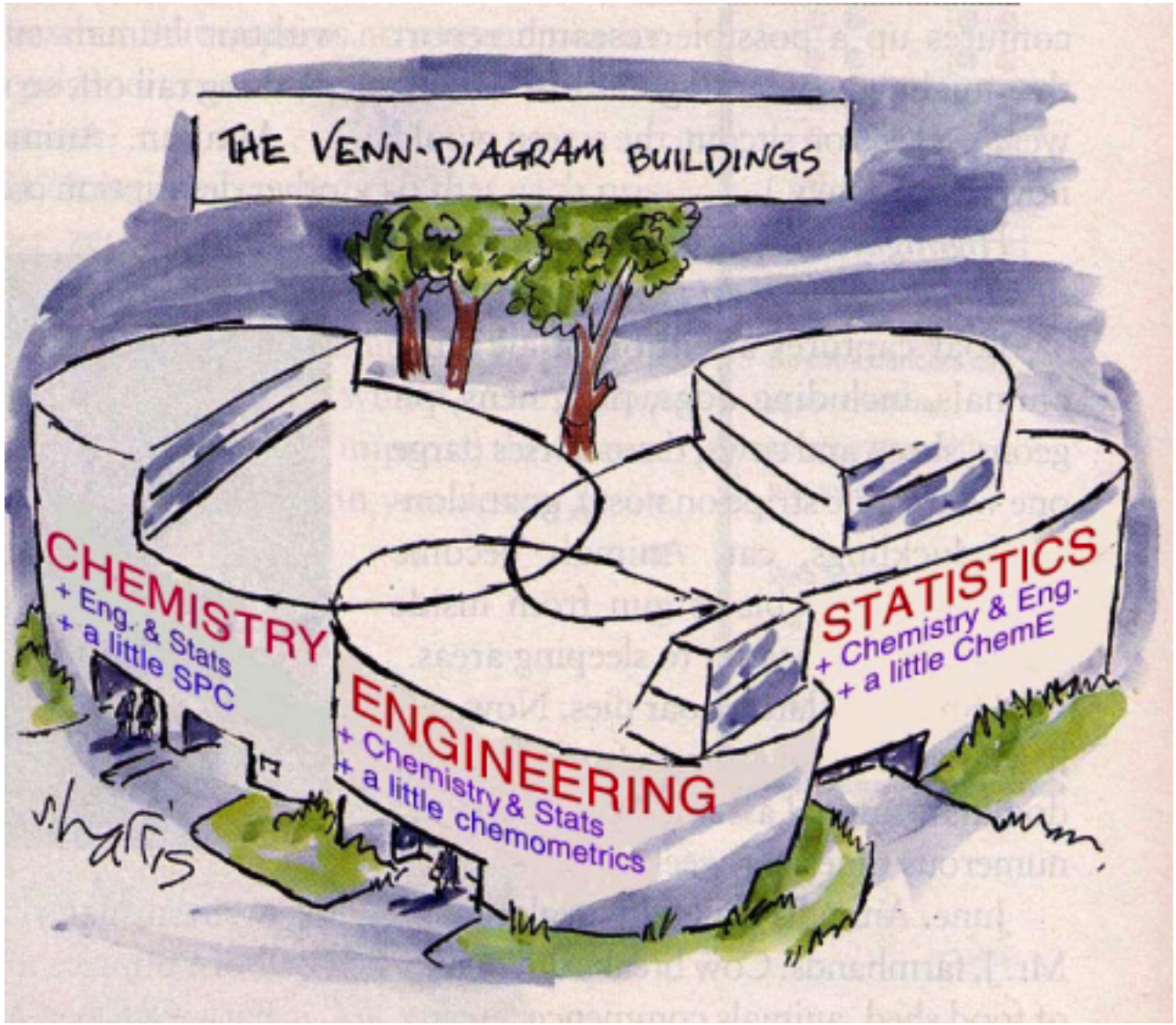

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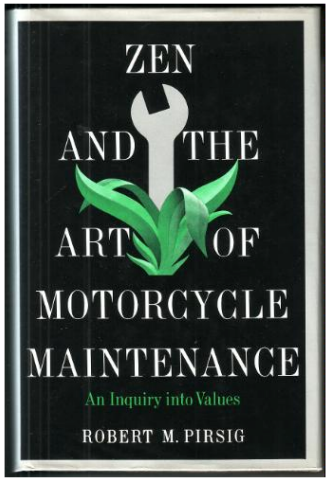
Outline

- General principles of SPC and fault detection
- Batch Chemical Processes
- Roadblocks
- Models
- The Roadmap
- Example: Comparison on Dupont Data
- Conclusions

General Principles of Fault Detection

- Process monitoring / Fault Detection / Statistical Process Control / Multivariate SPC / Batch SPC...
- Methods rely on a model that describes normal and/or desirable* operation
  - New data compared with model of "normal" data
  - Often much is learned from this model and the process of creating it!
  - Data considered normal to the process is likely not the same data useful for constructing regression models.



* Quality isn't JUST what you like, it IS what you like.
-Robert M. Pirsig, "Zen and the Art of Motorcycle Maintenance," William Morrow & Co. 1974

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Different Modeling Approaches

- Theoretical
  - Mathematical models, constructed from first principles
  - Applicable to information-sparse systems
    - good given satisfactory models and sufficient sensors
    - often time consuming to develop models
    - difficult to apply to large scale systems
- Empirical
  - Derived directly from process data
  - Applicable to data-rich systems
    - requires some redundancy in the data (fewer states than measurements)
    - highly dependent upon the quantity, quality and reliability of process instruments

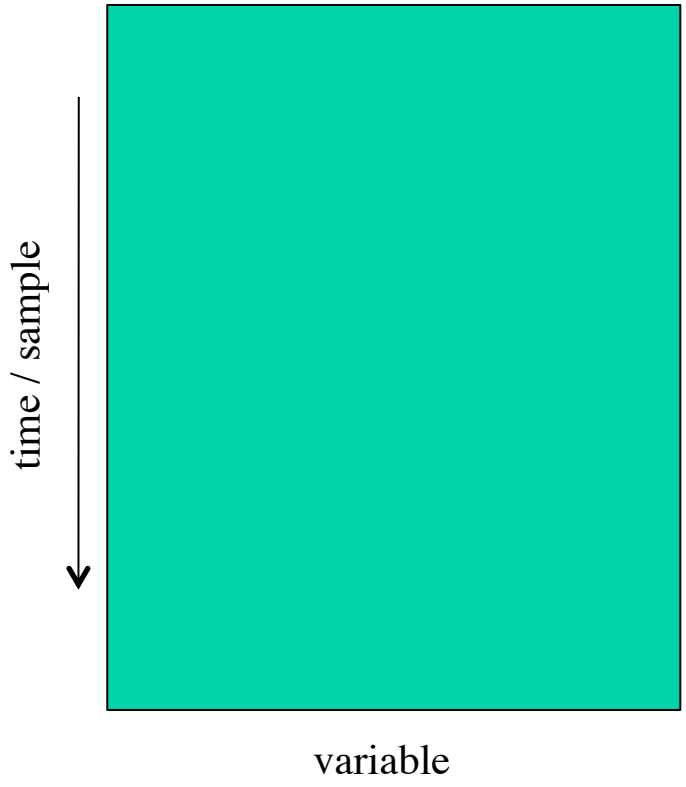
General Principles of Fault Detection

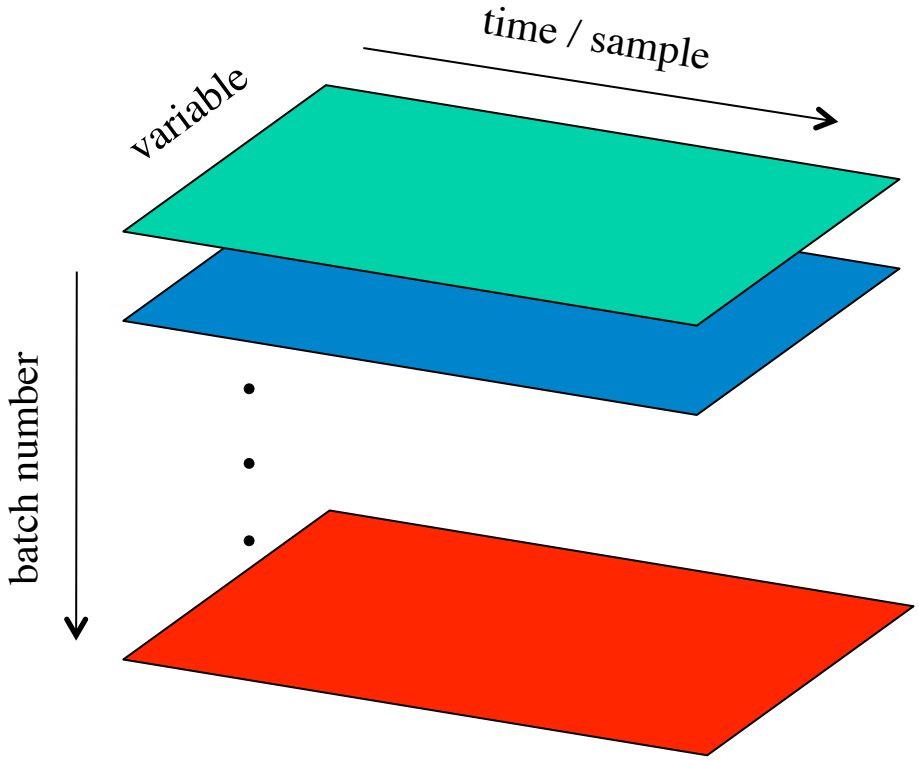
- Operating data is compared to the process model to determine if the process condition is nominal
  - do the new measurements look like the old ones or are they significantly different?
  - is the process in control?
- If different, it is useful to have diagnostic information about how it may be different
  - why is the process out of control?
  - some models are very good at providing diagnostics

Batch Chemical (and Manufacturing) Processes

- Many things made in batch (as opposed to continuous) processes:
  - Pharmaceuticals, enzymes
  - Food (cheese, yogurt), beverages (beer, wine)
  - Semiconductors
  - Polymers
  - etc....
- Batch data nominally 3-way
  - Process measurements (sensors, spectroscopy)
  - Batch running time
  - Batch number

Batch Data





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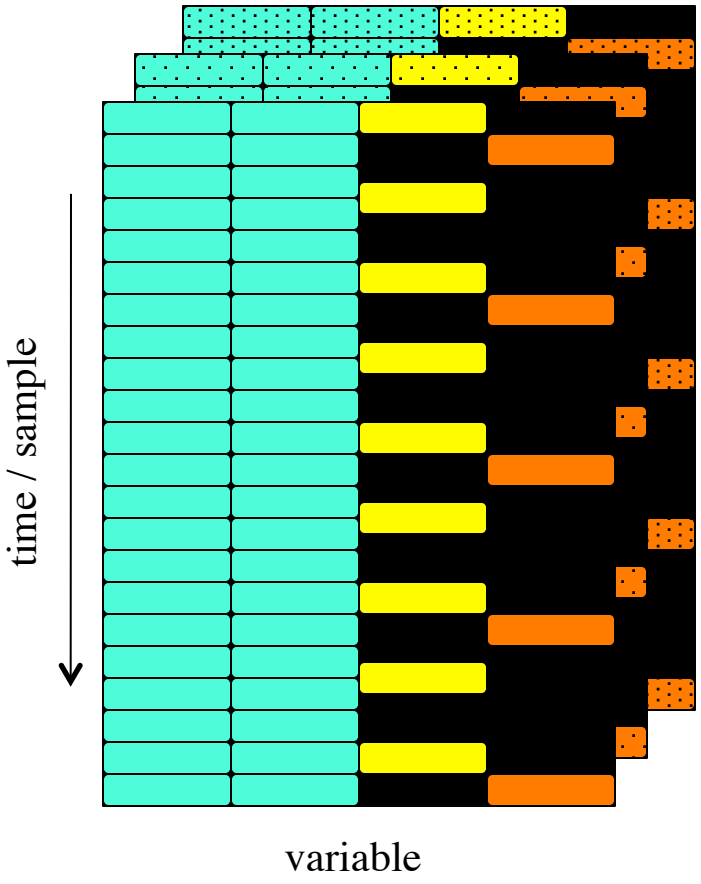
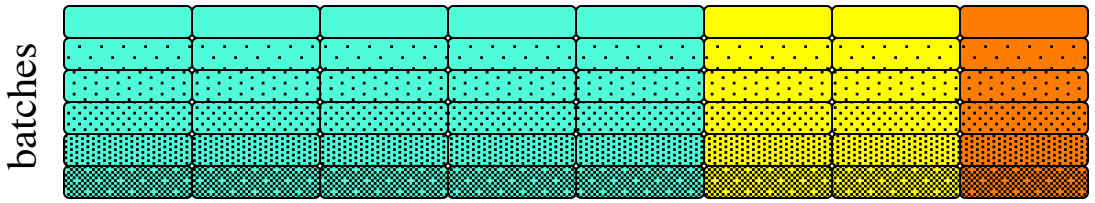
Different sample rates



- How to handle?
  - Zero order hold
  - Interpolate
  - Treat as missing?
- Doesn't matter in MPCA as long as it is consistent!



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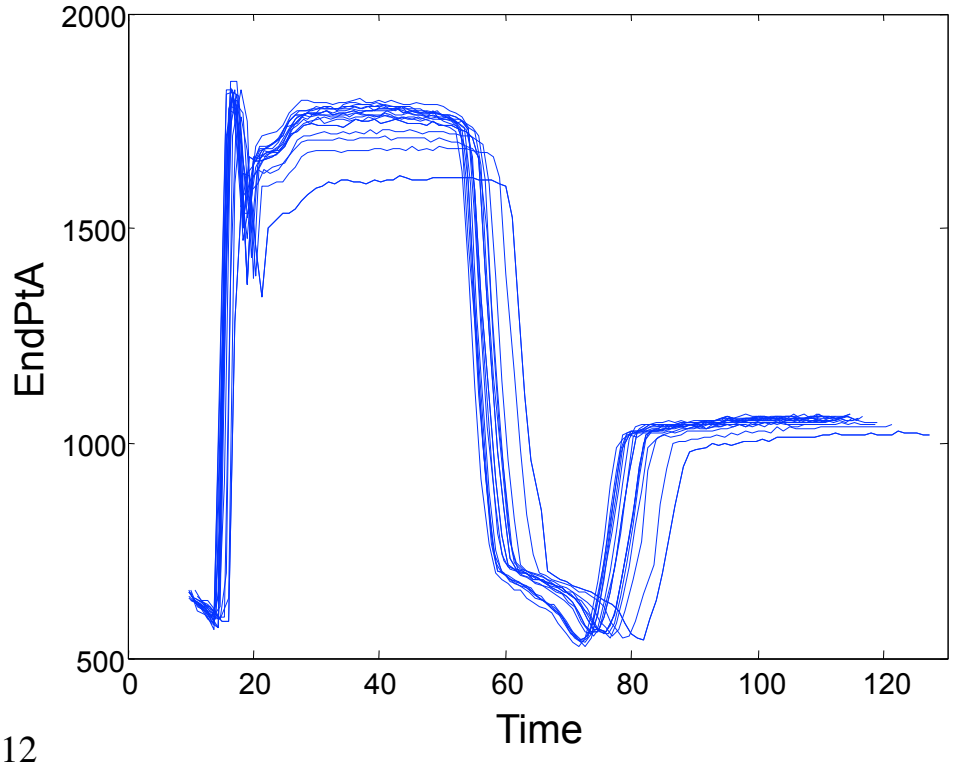
Batch Process Monitoring Data Problems

- The objective is to monitor batch-to-batch, but
  - data can be messy
    - typically includes start-up and shut-down phases that are not of interest
    - might be interesting if monitoring controller performance
  - periods of "steady-state" where not much is changing
  - variable record lengths
  - lots of data!
- Reduce to a set of more compact descriptors?
  - show an example…

Process Data Alignment and Dilation

- Batches "mature" at different rates
- Leads to files of different length
- Important transitions occur at different times



- Misalignment adds rank irrelevant to process monitoring.
  - model must account for time shifts in the process data.
  - Irrelevant variance often results in a reduction of model sensitivity.

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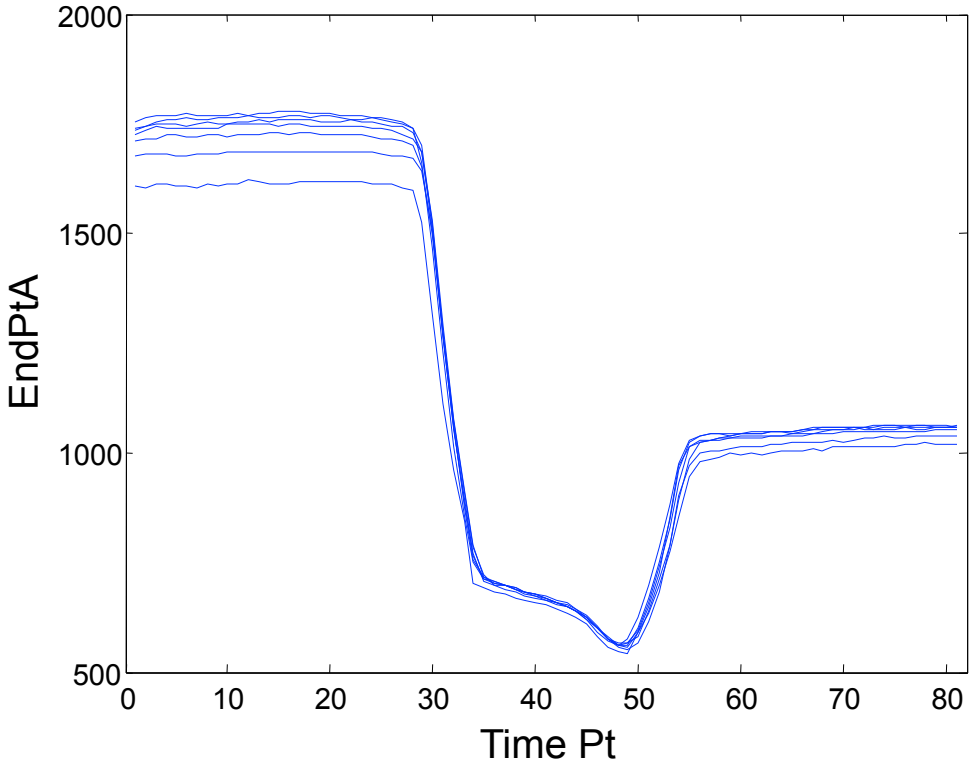
Aligned Process Data

- Many ways to align and/or warp
  - Align and truncate
  - Correlation Optimized Warping (COW)
  - Dynamic Time Warping (DTW)



Alternative:
Summarize data
over process steps

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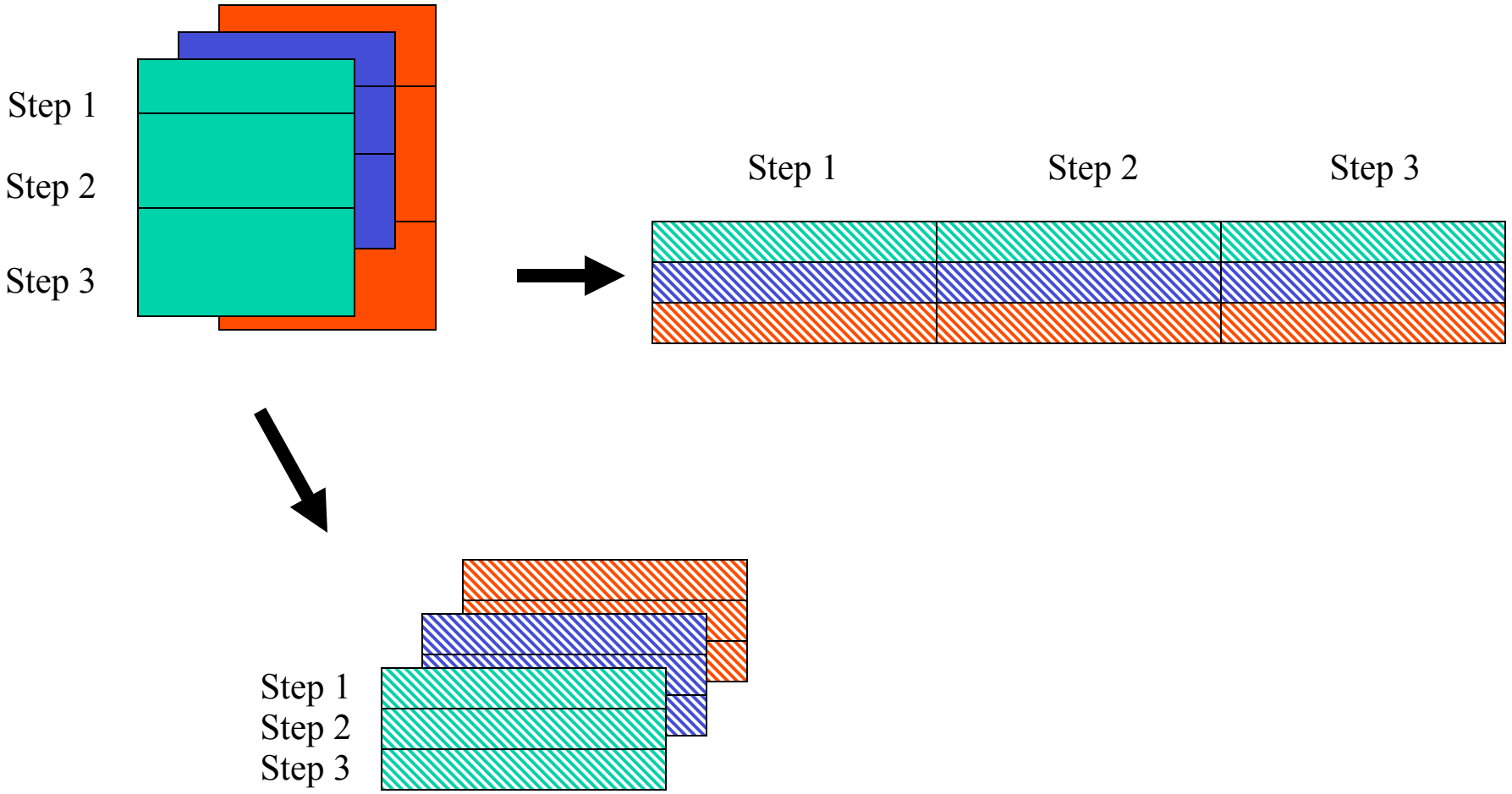
Data Summary Approach

- Convert data into alternate set of descriptors
- If process has multiple steps, calculate parameters that describe each step
  - mean
  - standard deviation
  - slope
  - length (time) of the step
  - etc....

Summary Variables



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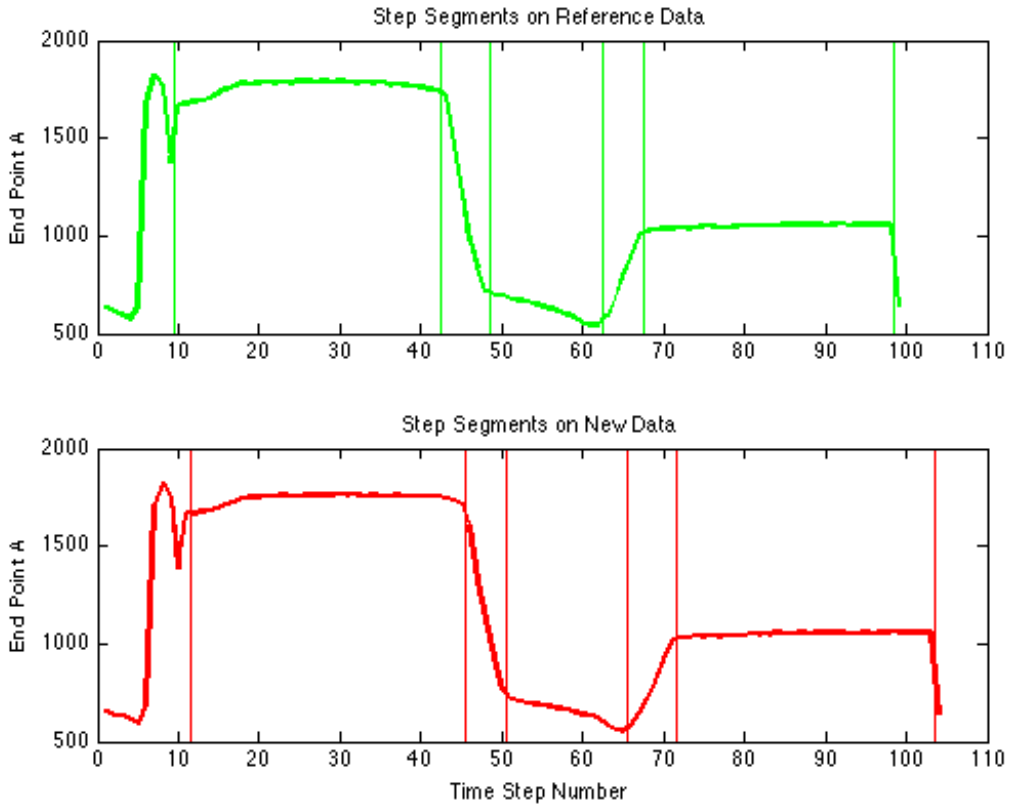
Summary Variables

- Pros
  - Conceptually simple
  - Some time information retained
  - Noise reduction
  - Reduces number of variables (vs. MPCA)
- Cons
  - Further from original data
  - May not have step numbers to work with

Creation of Pseudo-steps

- Several ways to do this
  - Manual assignment followed by warping
    - Break reference process variable into “sensible” segments (manually)
    - Assign step numbers
    - Warp new data onto reference
    - "Reverse warp" reference step numbers into new data
  - Automated peak picking
    - take first or second derivative of reference process variable
    - use peak peaking algorithm to find transitions

Example of Step Creation



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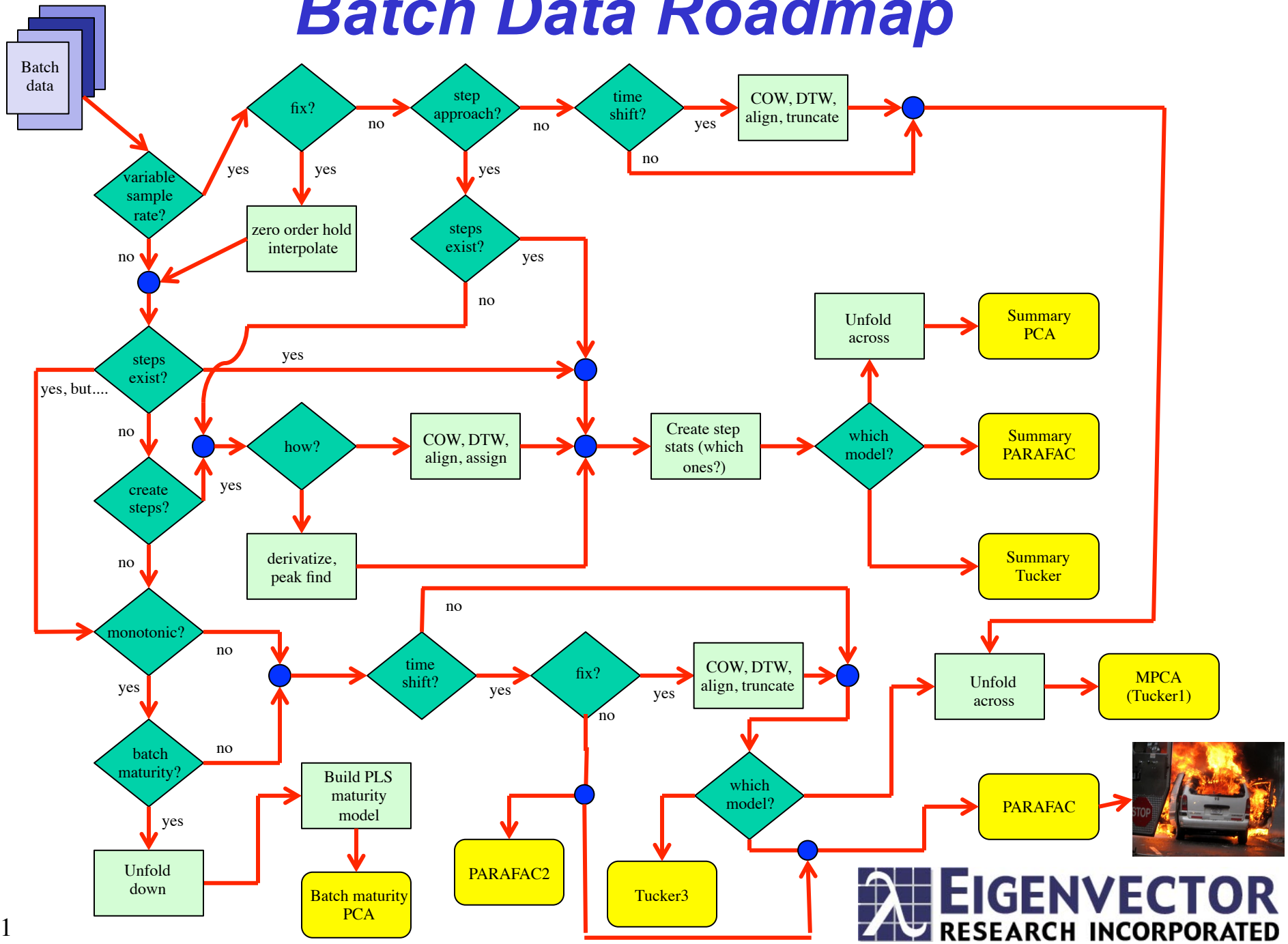
Batch Maturity Models

- Build PLS (or other) model that predicts extent of reaction or “batch time” for each time point
- Use model to predict where points should be on the time axis
  - can use as basis for warping, then can use PARAFAC, or MPCA model
  - use conventional PCA model (unfold down), make limits on scores, residuals etc. be a function of batch time

Which Model?

- Many to choose from!
  - MPCA (aka Tucker-1)
  - Summary PCA (MPCA on summary variables)
  - PARAFAC
  - Summary PARAFAC
  - PARAFAC-2
  - Tucker-3
  - Summary Tucker-3
  - Batch Maturity PCA
  - Tucker-2?

Batch Data Roadmap



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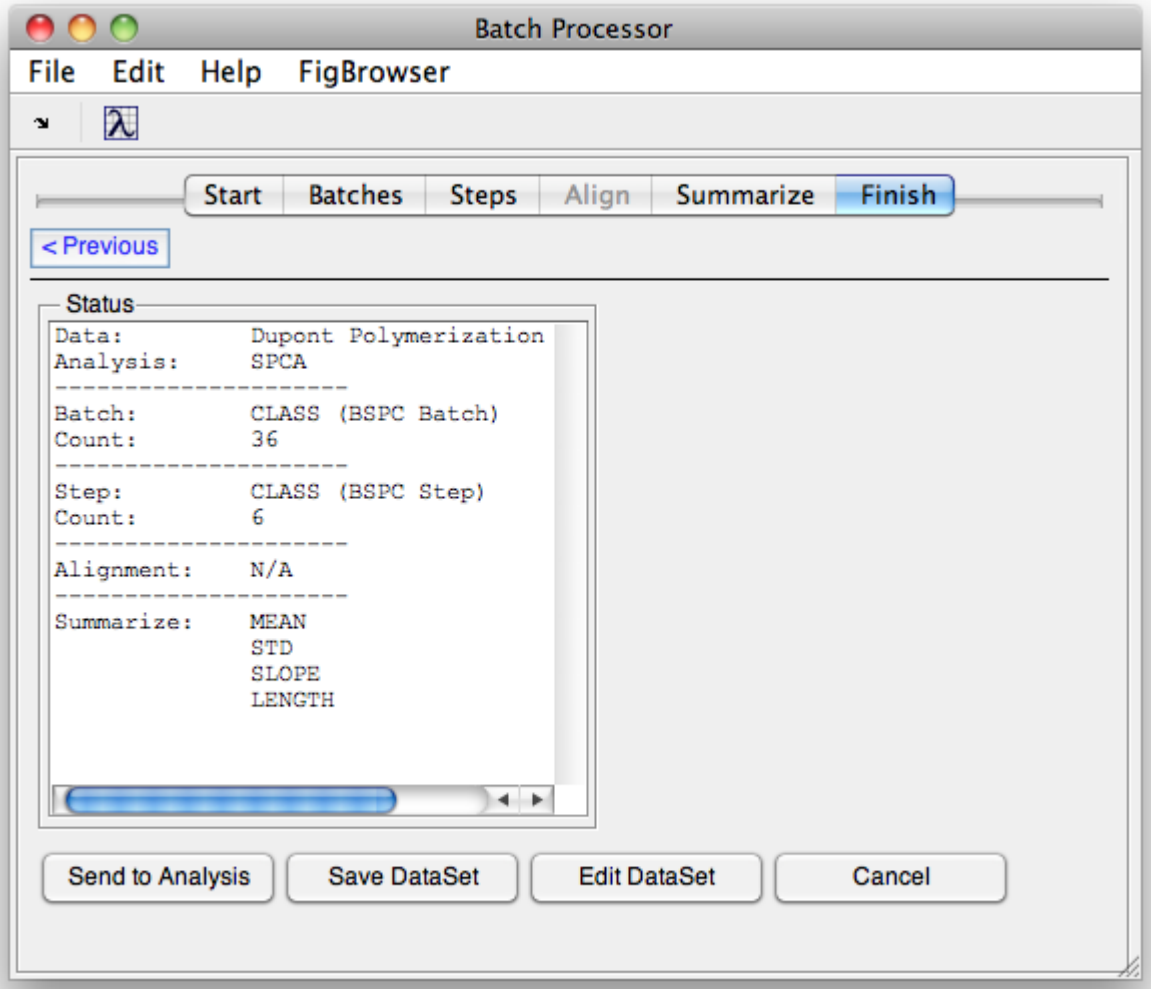
Batch Processor Tool



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Dupont Batch Data

- 10 process variables (sanitized)
  - 100 time intervals each
  - TempR 1, TempR 2, TempR 3, Press 1, Flow 1, TempC 1, TempC 2, Press 2, Press 3, Flow 2
- Calibration: 1 to 36 (normal batches)
- Test: 37 to 55 (one normal and seven faults)
  - Batches 40, 41, 42, 50, 51, 53, 54 and 55 had the final quality measurement well outside the acceptable limit
  - Batches 38, 45, 46, 49 and 52 were above or very close to that limit.
  - Batches 38, 40, 41 and 42 cannot be identified as abnormal batches.*
  - Additional batches 37, 39, 43, 44, 47, 47 and 48 were identified as somewhat unusual and were not included in the calibration set.*
- Described in

*Nomikos, P. and J.F. MacGregor, "Multivariate SPC charts for monitoring batch processes," Technometrics, **37**(1), 1995.

Methods

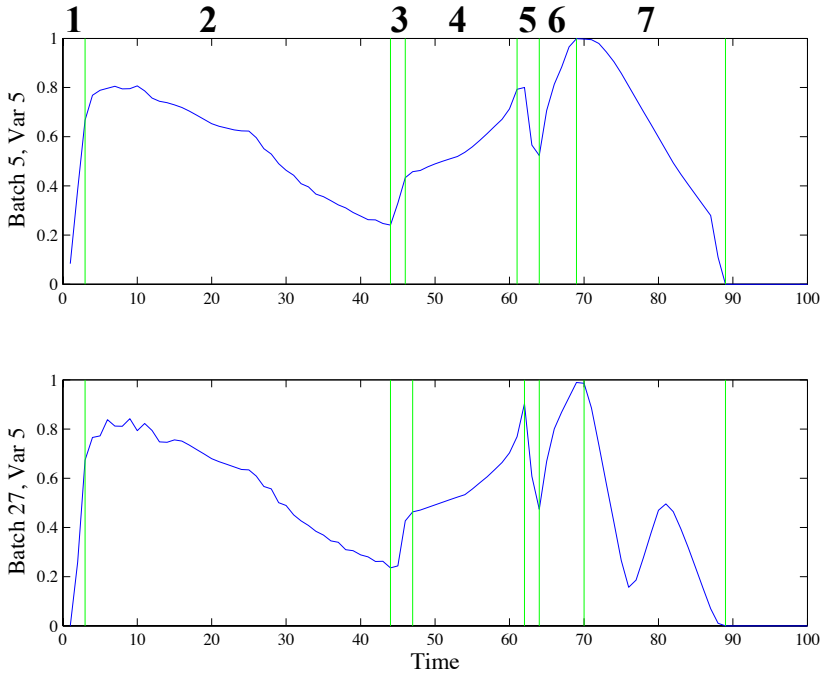
- Multi-Way PCA (MPCA, Tucker1)
  - block/group scaling on raw data
  - after COW
- Summary PCA (SPCA)
- Summary PARAFAC
- PARAFAC
- Batch Maturity PCA

SPCA

- PCA for summary variables
  - used steps 2-7
  - summarized by mean and step length
  - total variables = 10 * 6 + 6 = 66

Variable 5 is a feed flow and can be used to identify steps

Steps for two example batches



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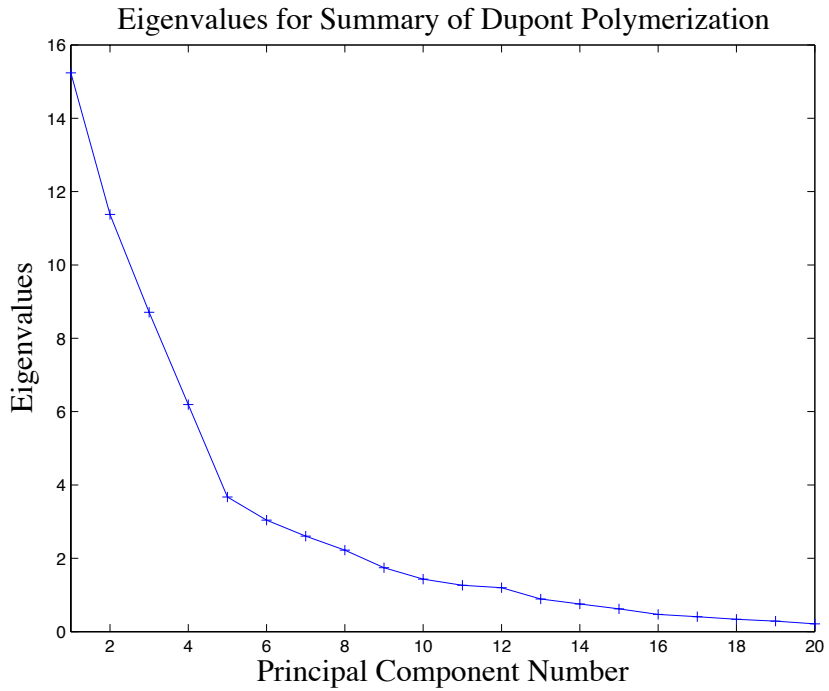
SPCA Variance Captured

```
X-block: Summary of Dupont Polymerization 36 by 64
Included: [ 1-36 ] [ 1-53 55-64 66 ]
Preprocessing: Autoscale
Num. PCs: 4
```

Percent Variance Captured by PCA Model

Principal Component Number	Eigenvalue of Cov(X)	% Variance Captured This PC	% Variance Captured Total
1	15.2	23.81	23.81
2	11.4	17.78	41.59
3	8.71	13.61	55.20
4	6.19	9.67	64.87



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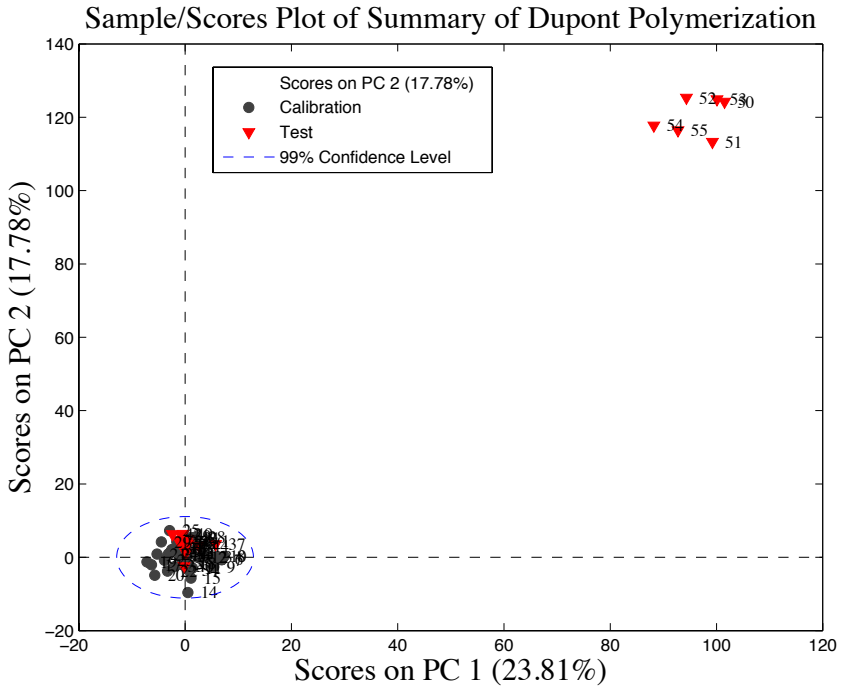
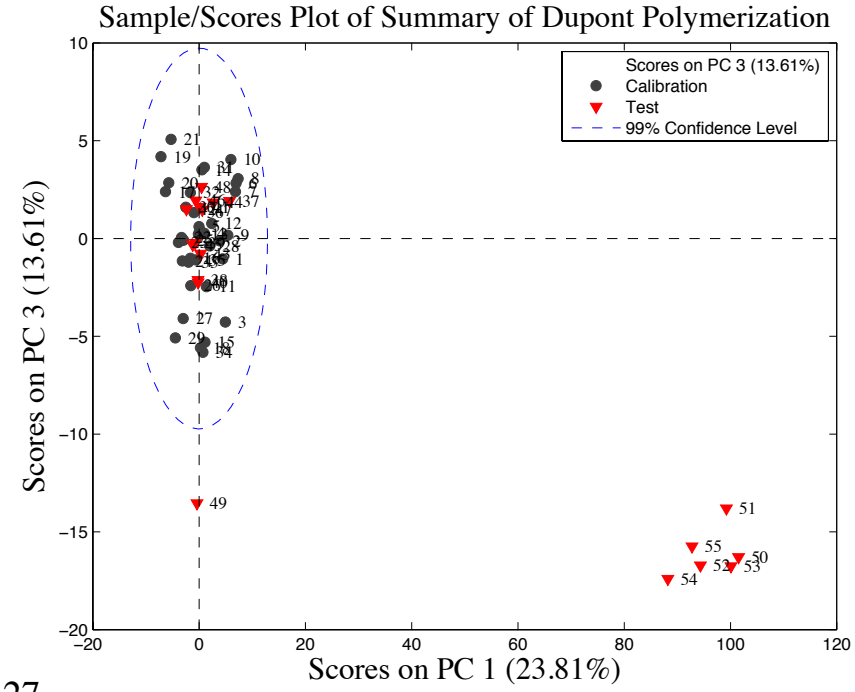
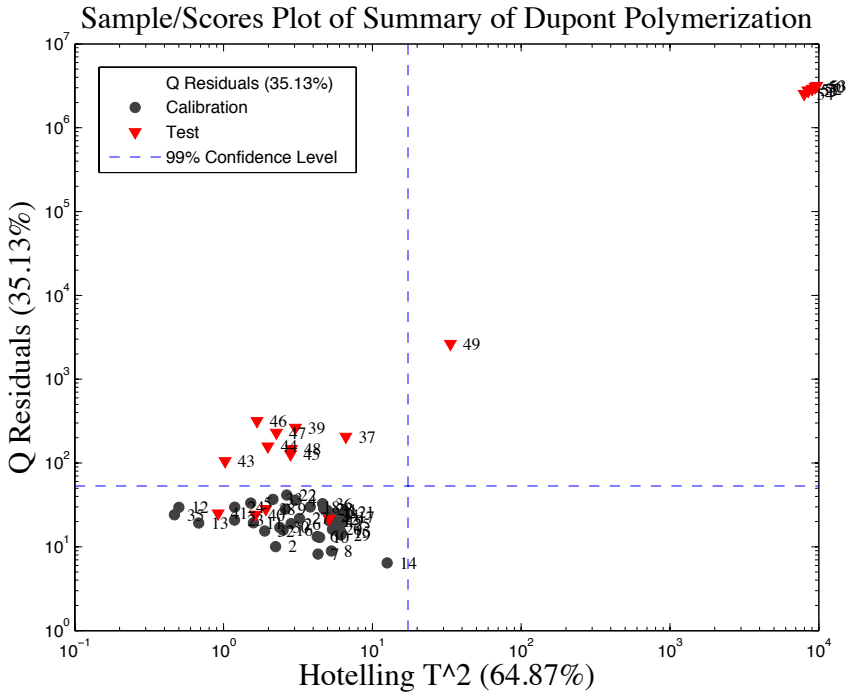
SPCA Scores







Out on both: 49, 50-55
Out on Q only: 37, 39, 43-48
Total coefficients: 4x66 = 264

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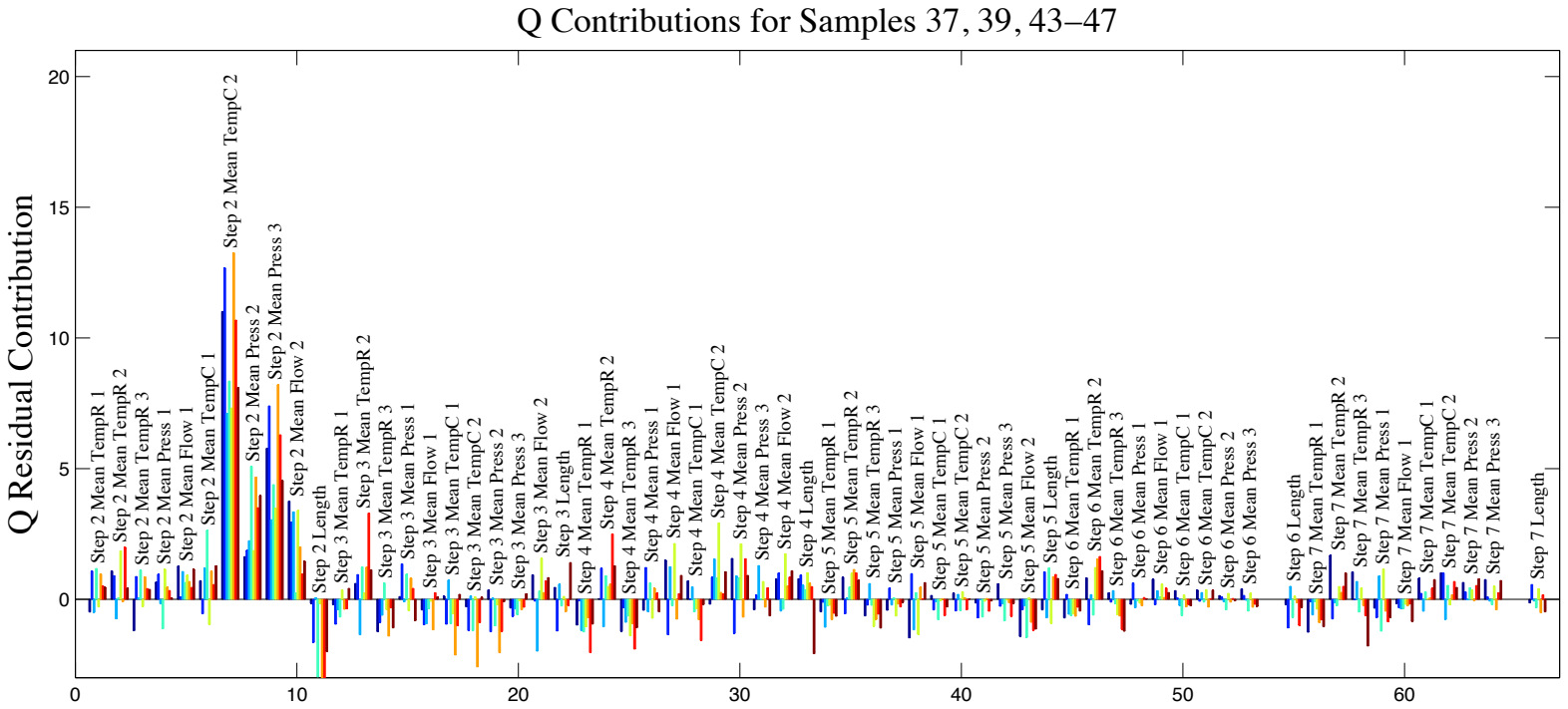
Varcap, Q Contributions



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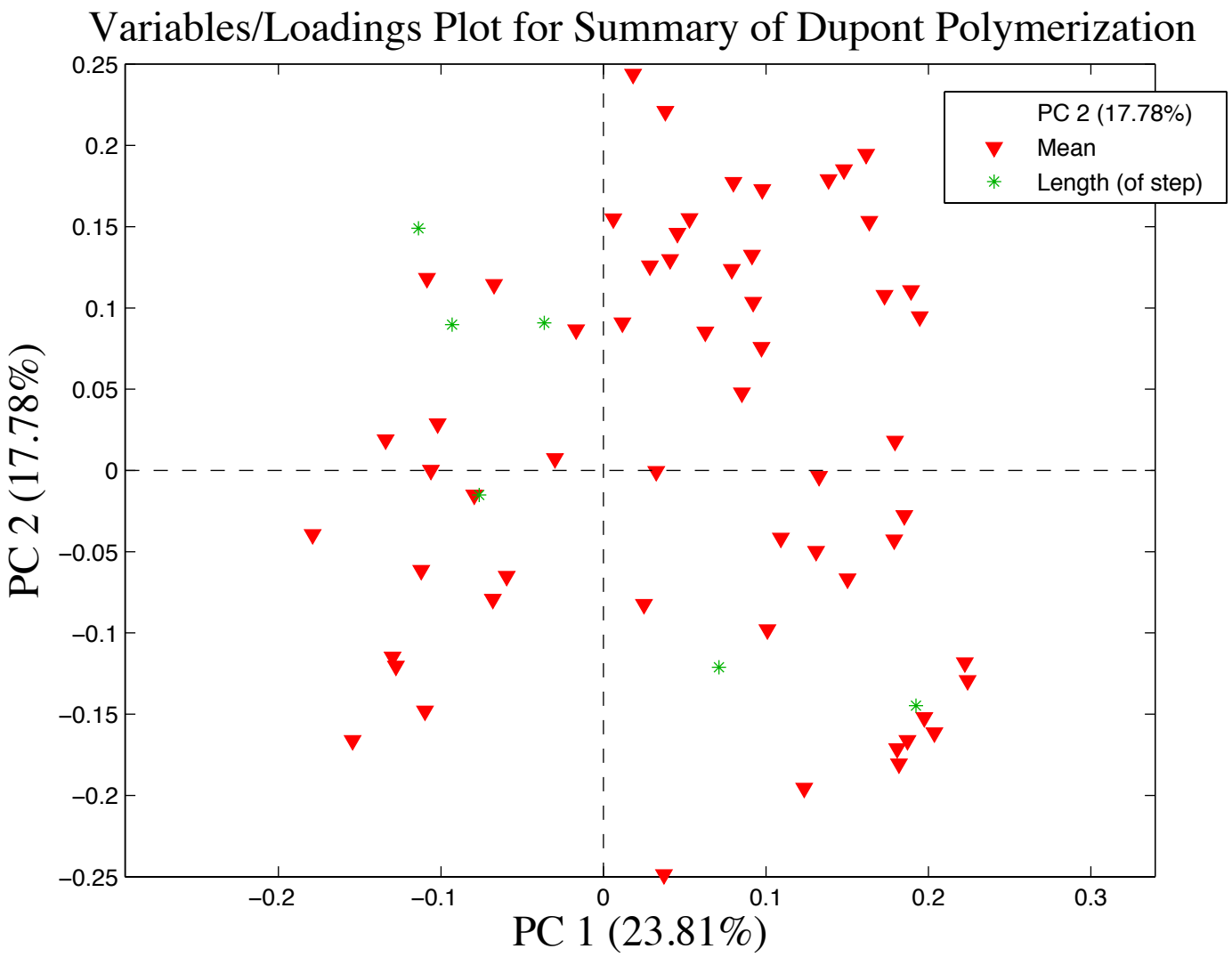
Loadings



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MPCA on Original Data

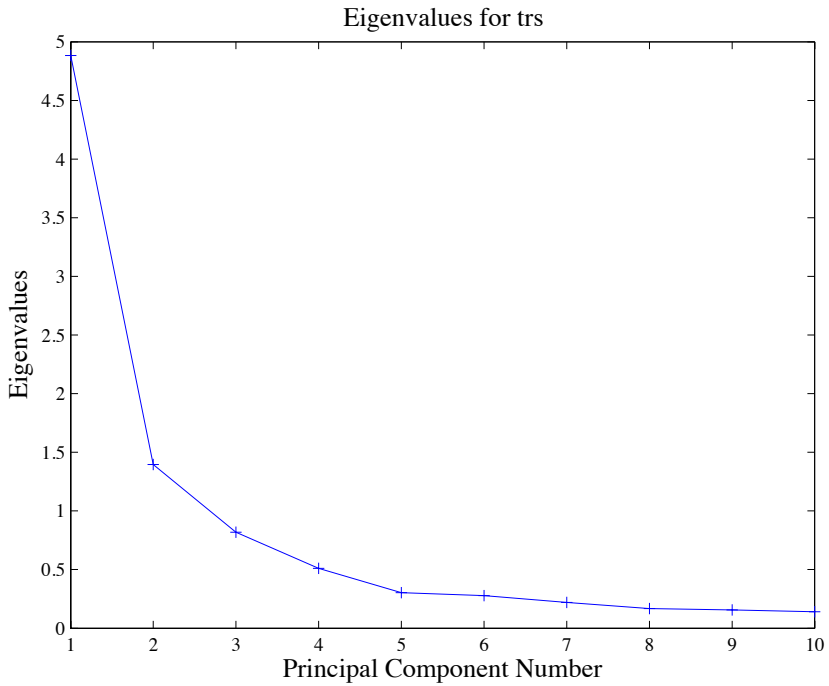
- MPCA with block scaling
- 100 time steps x 10 variables = 1000
- scale each block of the 100 new variables corresponding to individual original variables to unit variance and zero mean

MPCA Variance Captured

X-block: 47 by 1000
Preprocessing: Groupscale
Num. PCs: 3

Percent Variance Captured by PCA Model

Principal Component Number	Eigenvalue of Cov(X)	% Variance Captured This PC	% Variance Captured Total
1	4.88e+00	48.83	48.83
2	1.40e+00	13.95	62.78
3	8.19e-01	8.19	70.97



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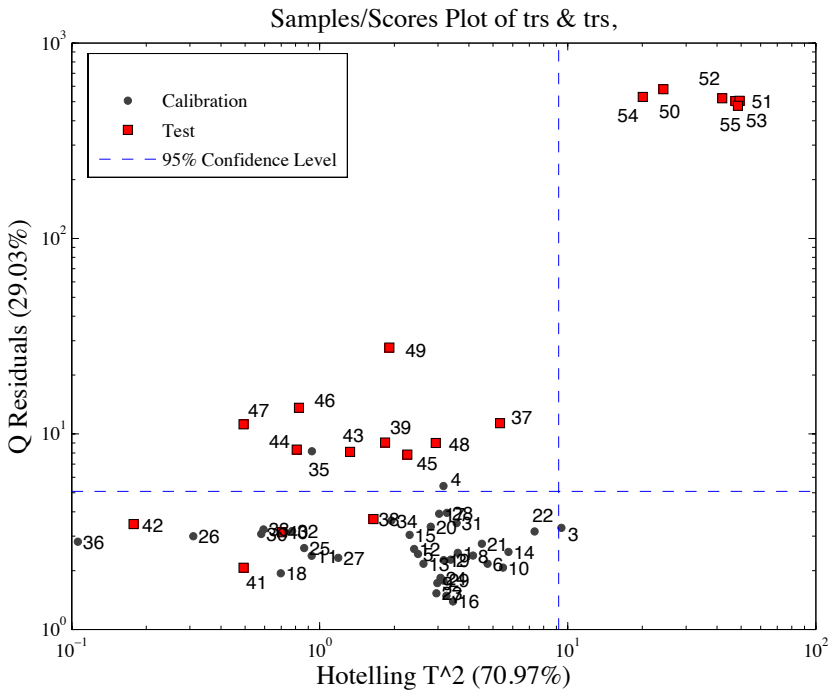

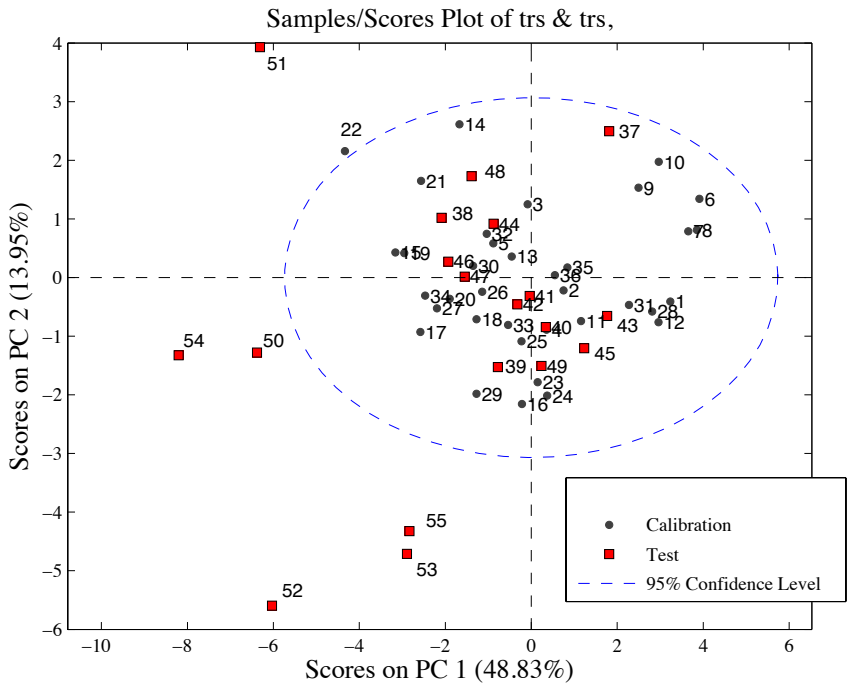

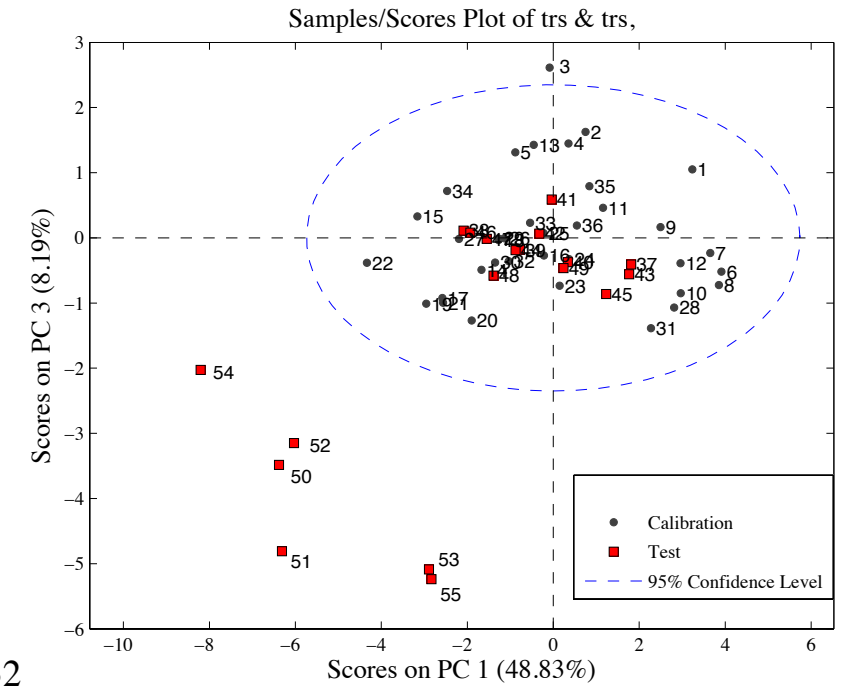

Out on both: 50-55
Out on Q only: 37, 39, 43-49
Total coefficients: 3x1000 = 3000!

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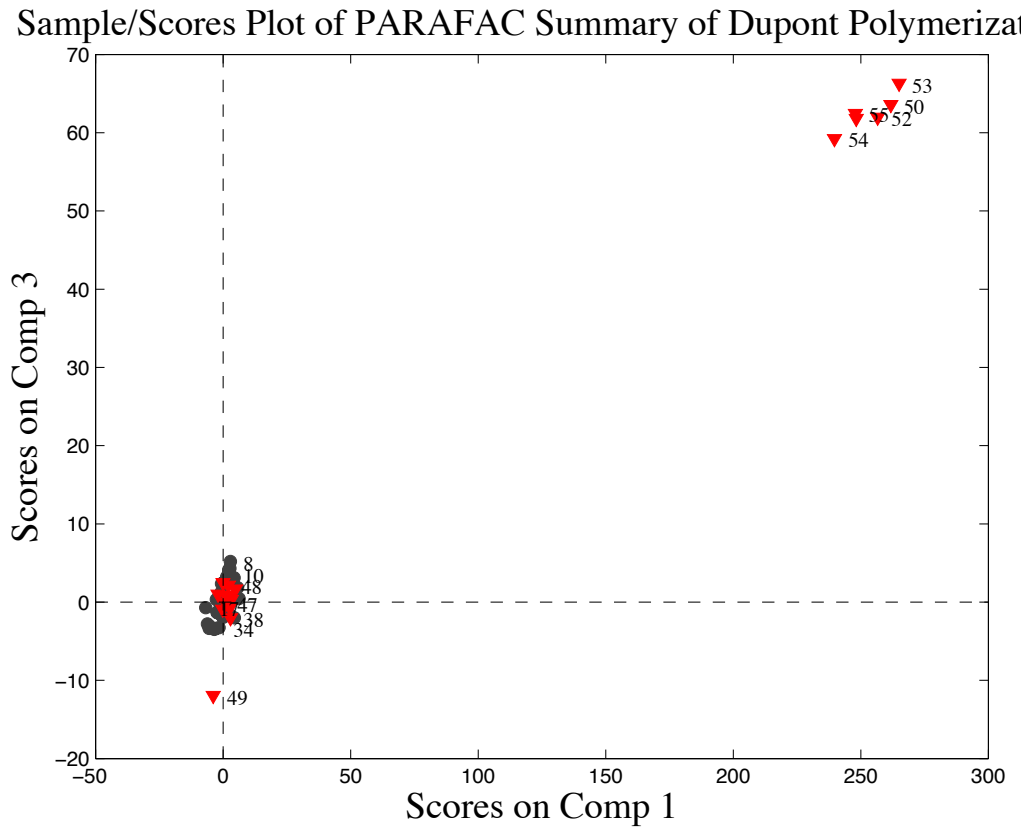
Summary PARAFAC



Out on both: 49-55
Out on Q only: no additional
Total coefficients:
3x11 + 3*6 = 51

Not as sensitive as SPCA and MPCA, but far fewer parameters

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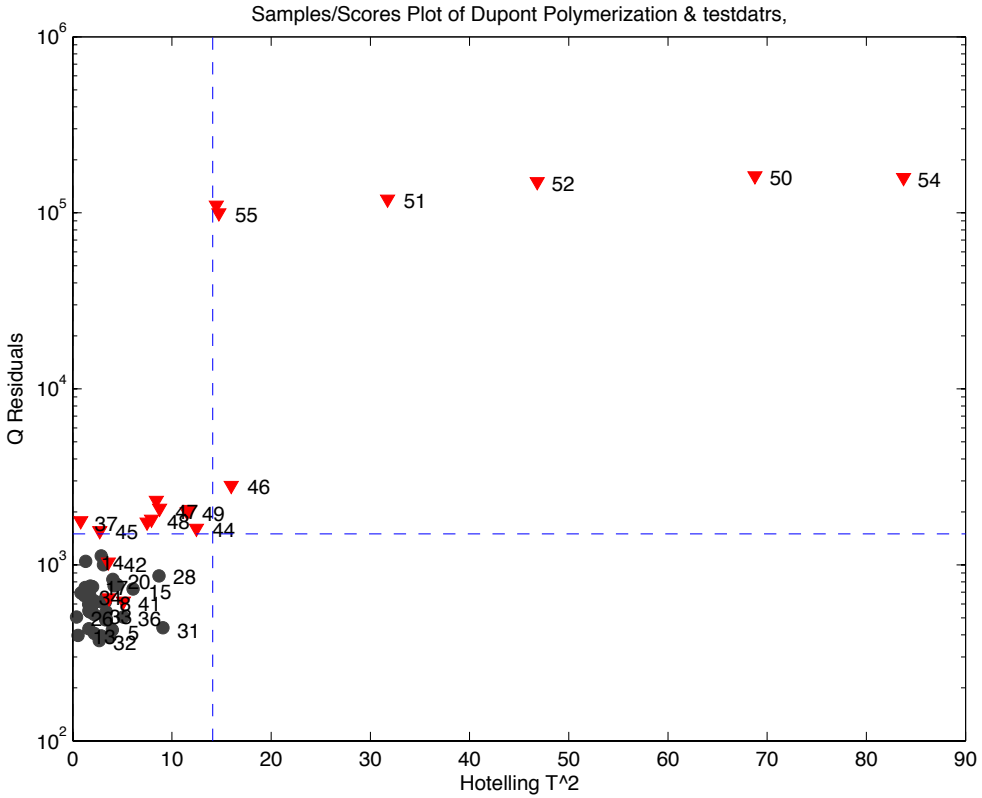
PARAFAC on Original Data



Out on both: 46, 50-55
Out on Q only:37, 39, 43-45, 47-49

Total coefficients:
3x10 + 3*100 = 330

Virtually same results as SPCA and MPCA

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Issues?

- Plenty!
- MPCA models easy to overfit, PARAFAC models sometimes not flexible enough
- Have not addressed run time application of models to partial batches
  - not so tough IF warping or step creation isn't an issue...
  - but hard to warp partial batches
  - some models can't be fit to partial data records (PARAFAC2)

Conclusions

- Too many options!
- Hard to know what method is best for particular application
- Challenging to implement in software that mere mortals can use
- If multi-way methods are to be adopted for batch processes, needs to be streamlined