Getting to Multiway: A Roadmap for Batch Process Data

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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
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
Different sample rates

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

Step 1
Step 2
Step 3

Step 1
Step 2
Step 3
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
**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

Batch data

variable sample rate?

yes

zero order hold interpolate

no

interpolate

steps exist?

yes

COW, DTW, align, assign

no

derivatize, peak find

steps exist?

yes

COW, DTW, align, assign

no

time shift?

yes

create steps?

yes

how?

no

COW, DTW, align, assign

yes

Unfold across

variable sample rate?

no

Batch maturity?

yes

Build PLS maturity model

no

time shift?

yes

fix?

no

COW, DTW, align, truncate

yes

Unfold across

PCA

which model?

PARAFAC

Summary Tucker

Summary PARAFAC

Summary PCA

MPCA (Tucker1)

monotonic?

no

batch maturity?

yes

Unfold down

no

Batch maturity PCA

yes, but....

variable sample rate?

no

interpolate

steps exist?

yes

COW, DTW, align, assign

no

derivatize, peak find

steps exist?

yes

COW, DTW, align, assign

no

time shift?

yes

fix?

no

COW, DTW, align, truncate

yes

Unfold across

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

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<th>Percent Variance Captured by PCA Model</th>
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<td>Principal Component Number</td>
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<tr>
<td>---------------------------</td>
</tr>
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<td>Principal Component Number</td>
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<tr>
<td>1</td>
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<td>2</td>
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<td>3</td>
</tr>
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<td>4</td>
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SPCA Variance Captured

Eigenvalues for Summary of Dupont Polymerization
Sample/Scores Plot of Summary of Dupont Polymerization

Scores on PC 2 (17.78%)
- Calibration
- Test
- 99% Confidence Level

Scores on PC 3 (13.61%)
- Calibration
- Test
- 99% Confidence Level

Sample/Scores Plot of Summary of Dupont Polymerization

Scores on PC 1 (23.81%)

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

Variables/Loadings Plot for Summary of Dupont Polymerization

PC 1 (23.81%)
PC 2 (17.78%)

Mean
Length (of step)
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

<table>
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<th>Cov(X)</th>
<th>This PC</th>
<th>Total</th>
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<tbody>
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<td>48.83</td>
<td>48.83</td>
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<td>2</td>
<td>1.40e+00</td>
<td>13.95</td>
<td>62.78</td>
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<td>3</td>
<td>8.19e-01</td>
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</table>

Eigenvalues for trs

![Eigenvalues Plot]
Out on both: 50-55
Out on Q only: 37, 39, 43-49
Total coefficients: $3 \times 1000 = 3000!$
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
**PARAFAC on Original Data**

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

Total coefficients:  
$3 \times 10 + 3 \times 100 = 330$

Virtually same results as SPCA and MPCA
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