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Supply Chain Monitoring using Multivariate Statistical Analysis

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Acknowledgements

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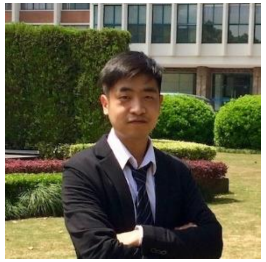

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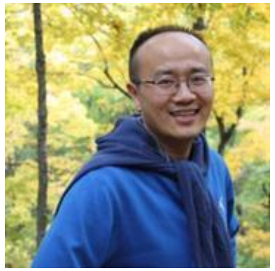

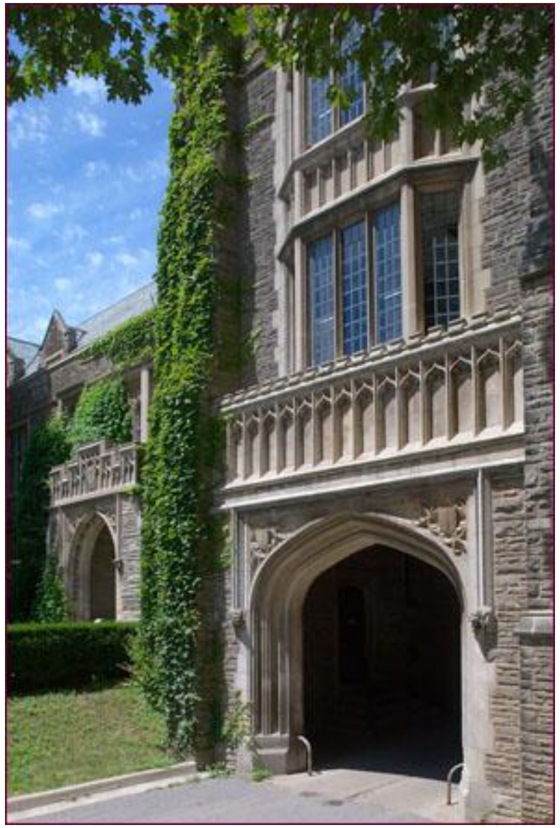

Brandon Corbett

MacData Institute

MacDATA INSTITUTE

McMaster Advanced Control Consortium

MACC McMaster Advanced Control Consortium

ProSensus data driven innovation

Outline

- Introduction
  - Supply chain monitoring
- Principle Component Analysis (PCA)
  - Overview & monitoring tools
  - Supply chain monitoring using PCA
  - Supply chain simulation
  - Case studies
- Canonical Variate Analysis (CVA)
  - Overview & monitoring tools
  - State space formulation of supply chain operation
  - Supply chain monitoring using PCA
  - Case studies
  - Fault impact prediction
- Conclusions

Introduction

- A well-functioning supply chain is **critical to the overall profitability** of a manufacturing enterprise
- Supply chain **disruptions** could lead to significant economic loss without a **timely detection** and an **effective mitigation strategy**

GE.com/GettyImages

Focus of this study

- **Detection and identification of abnormalities** in supply chain operation using techniques of multivariate statistical analysis

Supply Chain Monitoring (SCMo)

- Research on SCMo involves contributions from a variety of domains.
- Use of multivariate statistical methods in SCMo is scant.

Articles	Supply chain data/KPIs	Models/methods	Journals/conferences
Lau et al. (2002)	Delivery time, product quality	A fuzzy logic model	Logistics Information Management
Bansal et al. (2005)	Stock inventory, throughput	Causal models	Computer Aided Chemical Engineering
Mele et al. (2005)	Material flows, orders, inventory levels	Multi-scale delay adjusted PCA	Computer Aided Chemical Engineering
Fei and Wang (2008)	Delivery delay, inventory levels	A recurrent neural network	International Symposium on Computer Science and Computational Technology
Chae (2009)	KPIs for plan, source, make, and delivery	Supply chain operations reference (SCOR) model	Supply Chain Management
Zhou and Rong (2010)	Customer needs	Integration definition for function modelling (IDEF0)	International Conference on Logistics Systems and Intelligent Management
Goh et al. (2013)	Logistics, inventory, order and manufacturing information, risk-related information	A supply chain visualization platform	IEEE International Conference on Automation Science and Engineering
Irizarry et al. (2013)	Status of materials	A supply chain visualization system	Automation in Construction
Fernández et al. (2015)	Orders and resources associated with a schedule	A multi-agent monitoring system	Computers in Industry
McKinney et al. (2015)	Containers	Container monitoring devices	Transportation Research Record
Blos et al. (2018)	Historical database of supply chain disruptions	Petri net and agent-based model	International Journal of Production Research

Principal Component Analysis (PCA)

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Development and Applications

- PCA is designed for extracting uncorrelated components from correlated data (Wold et al., 1987)

  Characteristic: dimensionality reduction

- PCA first formulated in statistics by Pearson (1901), and NIPALS algorithm outlined in Fisher and Mackenzie (1923)

- PCA-based statistical process modeling and monitoring (Kresta et al., 1991, Kourti and MacGregor 1995)

- Applications in the process system engineering community
  - statistical process monitoring: MacGregor et al. (2005), Qin and Chiang (2019)
  - dimensionality reduction: Ning and You (2018), Hassanpour et al. (2022)
  - optimization in the latent variable space: Flores-Cerrillo and MacGregor (2004), Golshan et al. (2009)

- Extensions of PCA include:
  - dynamic PCA (Ku et al., 1995)
  - kernel/nonlinear PCA (Lee et al., 2004)
  - dynamic inner PCA (Dong and Qin, 2018)

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Formulation

Data: $X_{N\times K} = [x_1, x_2, \ldots, x_N]^T$

x_i: K-dimensional vectors of data collected at time point i

PCA model: Projection of X onto lower-dimensional subspace spanned by columns of T

$$T = XP$$

$$X = TP^T + E = \sum_{a=1}^{A} t_a p_a^T + E$$

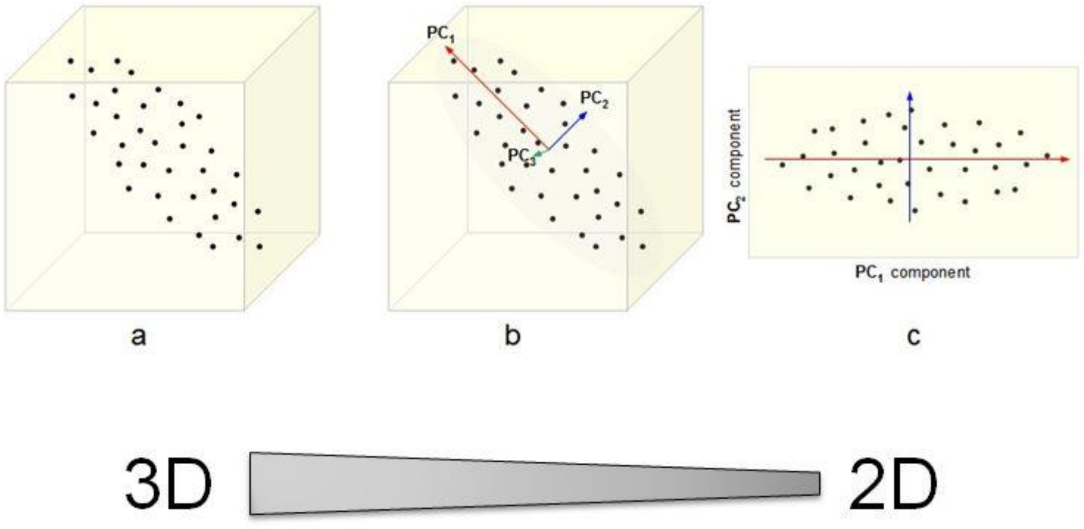
loading: $P = [p_1, p_2, \ldots, p_A]$

score: $T = [t_1, t_2, \ldots, t_A]$, $t_a = Xp_a$

residual: E

Compute via

- Eigendecomposition of sample covariance matrix $S = \frac{1}{N-1}X^TX$, or
- SVD on X
- Nonlinear partial least squares (NIPALS) algorithm



www.davidzeleny.net/anadat-r/doku.php/en:pca

Principal Component Analysis

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PCA-based process monitoring

- **Monitoring statistics & confidence limits**

Sample x_i can be projected to the principal component subspace (PCS) and the residual subspace (RS).

- PCS: Hotelling's T^2

$$T^2(x_i) = t_i^T D^{-1} t_i = x_i^T P D^{-1} P^T x_i \sim \chi^2(A)$$

where D is diagonal matrix of eigenvalues of S.

- RS: Squared prediction error (SPE)

$$SPE(x_i) = \|E_i\|_2^2 = \|x_i^T - t_i^T P^T\|_2^2 \sim \frac{v}{2m}\chi^2(\frac{2m^2}{v})$$

where $m = mean(SPE), v = var(SPE)$.

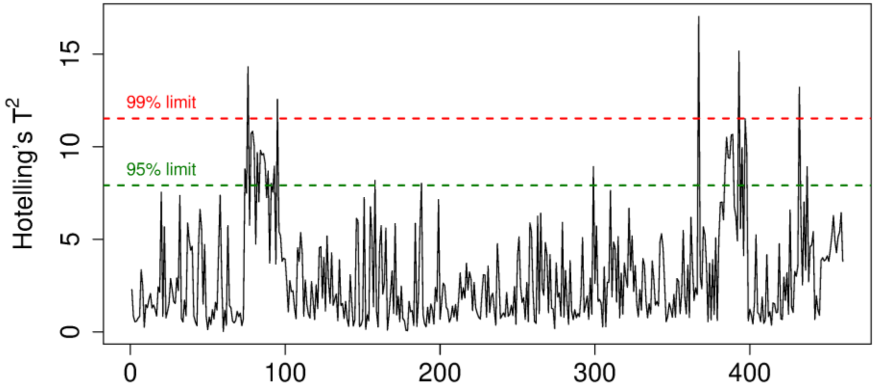
- **Fault detection**
  - Project the real-time data into PCS and RS:

$$t_i^T = x_i^T P$$
$$\tilde{x}_i^T = x_i^T - t_i^T P^T$$

  - Calculate monitoring statistics.
  - Raise an alarm if:

$$T^2(x_i) = t_i^T D^{-1} t_i \geq \chi_\alpha^2(A)$$
$$SPE(x_i) = \|\tilde{x}_i\|_2^2 \geq \frac{v}{2m}\chi_\alpha^2(\frac{2m^2}{v})$$

  - Example of monitoring chart



Kevin Dunn. Process Improvement Using Data. learnche.org/pid/

Principal Component Analysis

PCA-based process monitoring

- Fault diagnosis – identify fault-related variables

Contribution to t_a: $C_{a,j} = x_{ij} p_{aj}$
where

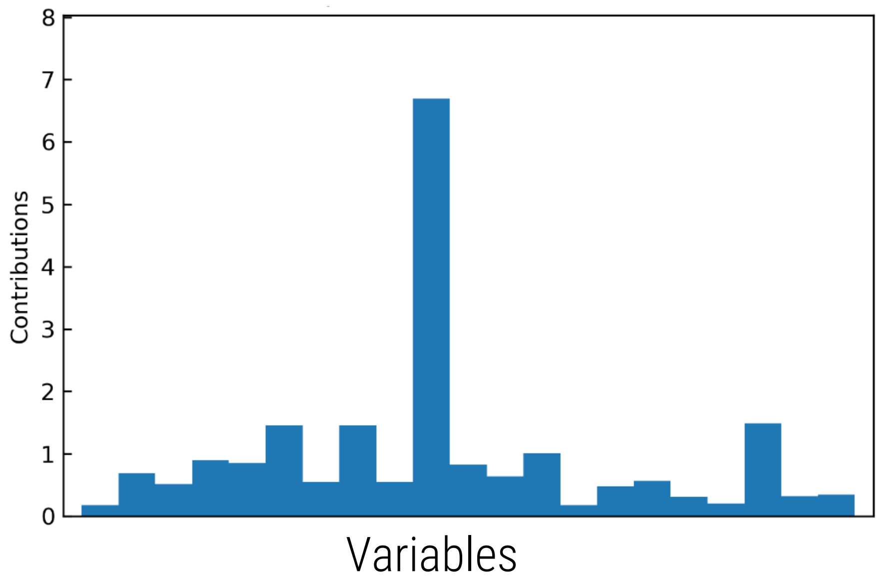
x_{ij} is the j-th entry of x_i

p_{aj} is the j-th entry of the a-th loading p_a

Contribution to SPE: $C_j = \tilde{x}_{ij}^2$
where

$\tilde{x}_{ij}$ is the j-th entry of the residual $\tilde{x}_i$

Example: contribution to SPE



- Dynamic PCA (DPCA)
  - Takes into account autocorrelation
  - PCA on augmented data

$$z_k = [x_k^T, x_{k-1}^T, \ldots, x_{k-l}^T]^T$$
$$Z = [z_{l+1}, z_{l+2}, \ldots, z_N]^T$$

Applications of PCA in Supply Chain Analytics

Articles	Applications of PCA
Mele et al. (2005)	Demonstrate the application of PCA techniques for detection of manufacturing and transportation delays in a simulated supply chain system. Their study includes a wavelet based multiscale PCA technique and a Genetic Algorithm based search scheme to account for time delays.
Lei and Moon (2015)	Use PCA to help determine market segments for new products and develop a decision support system for market-driven product positioning and design.
How and Lam (2018)	Use PCA to reduce the redundancies of performance indicators, thus aiding the multiobjective optimization of a supply chain.
Ning and You (2018) Gao et al. (2019)	Data-driven supply chain optimization: PCA is applied to help characterize uncertain parameters in a supply chain by reducing the dimensionality of the correlated uncertainty data.
Pozo et al. (2021)	PCA is employed to reduce the computational complexity of a multiobjective optimization problem formulated for supply chain design. Redundant metrics are identified and omitted while retaining the main features of the problem.

- Application of PCA to SCMo is scant.

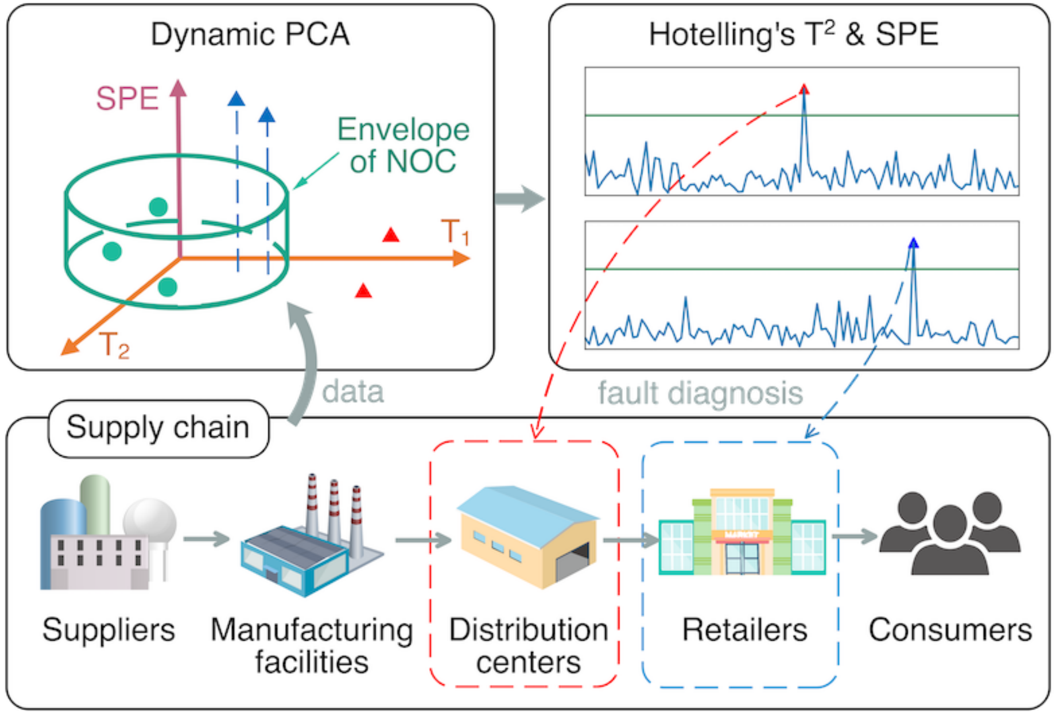
Data-driven SCMo Using PCA*

Training step

1. Collect NOC data of supply chain (inventory levels, products in transit, etc.)
2. Preprocessing: Augment data for DPCS; normalize data to have zero mean and unit variance.
3. Perform PCA/DPCA; obtain loadings and scores
4. Calculate the monitoring statistics (T^2 and SPE) of the NOC data
5. Determine the confidence limits of T^2 and SPE

Monitoring step

1. Normalize new data point with mean and standard deviation of each variable from training step.
2. Project new data into PCS and RS to obtain scores and residuals.
3. Calculate the T^2 and SPE of new data
4. Check whether the T^2 and SPE are both within their confidence limits. If abnormal operation detected, use contribution plots to identify fault-related variables.



*Wang, J., Swartz C.L.E., Corbett, B., and Huang, K. Ind. Eng. Chem. Res., 59(27):12487-12503, 2020.

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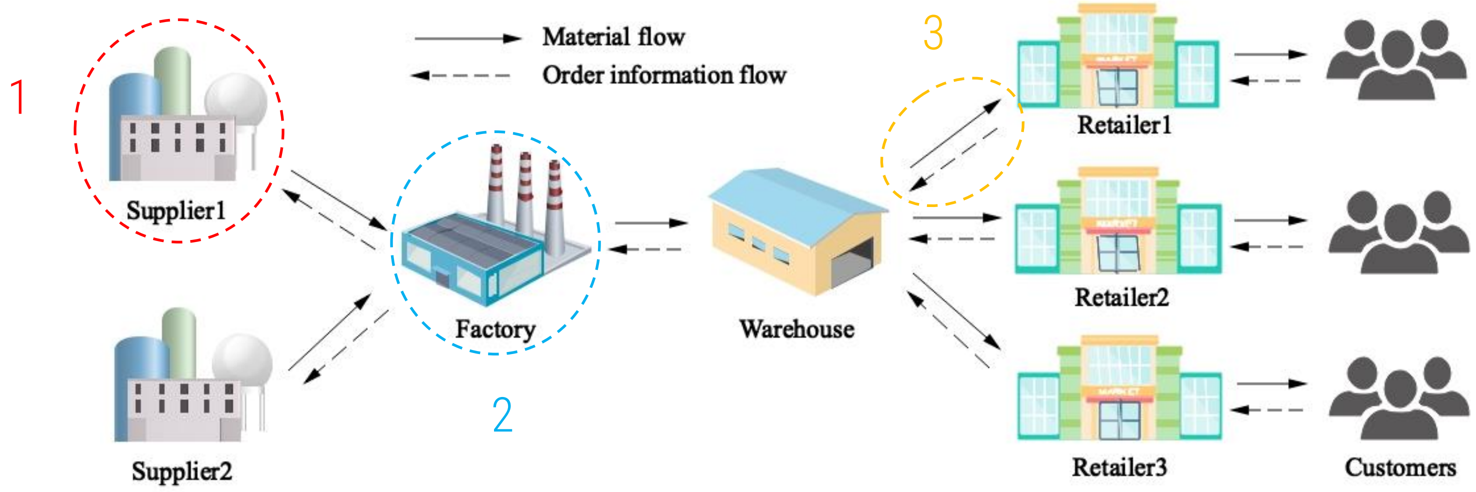
Case study I: A multi-echelon supply chain



Wang, J., Swartz C.L.E., Corbett, B., and Huang, K. Ind. Eng. Chem. Res., 59(27):12487-12503, 2020.

Fault scenarios:

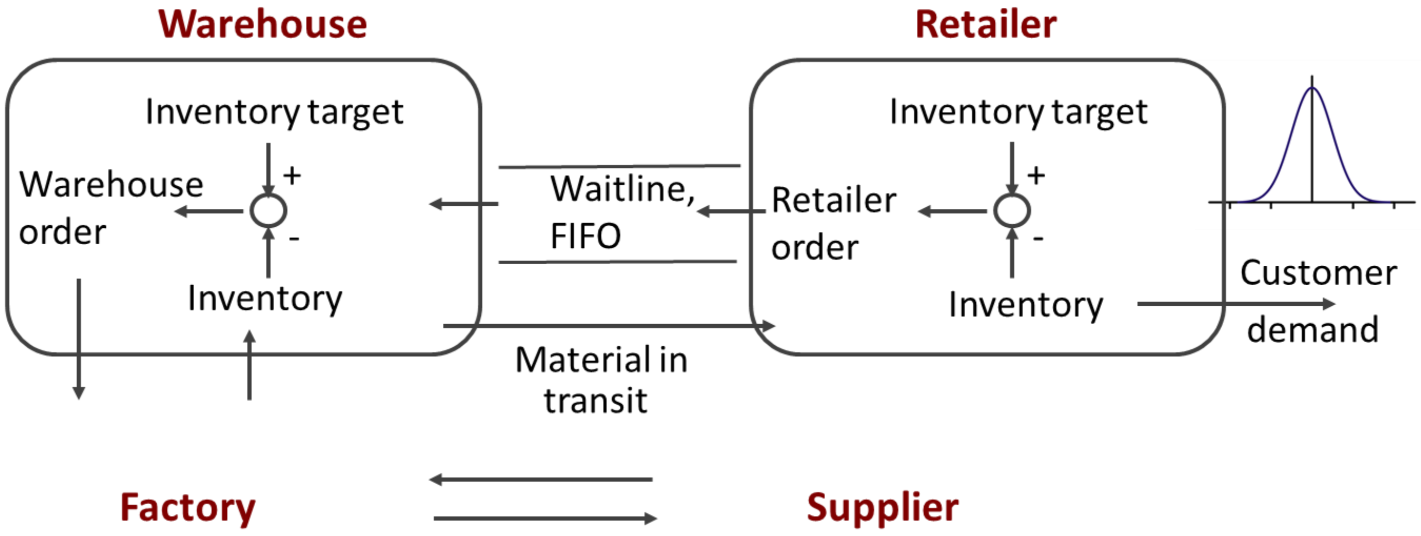
1. Raw material shortage - Supplier 1
2. Reduced yield
3. Transportation delay

- Raw materials M1 and M2 to produce product A: $0.5M1 + M2 \longrightarrow A$
- Inventory policy: (s, S), s – reorder point, S – target inventory
- Demand: multivariate Gaussian distribution
- Data for 21 variables: retailer and warehouse orders (4), inventory levels (9), products in transit or processing (8)
- Based on NOC data, 10 PCs explain 85% of variance for PCA; 18 PCs explain 82% of variance for DPCA with 2 lags.

Supply Chain Simulation

Supply chain simulation model

- Agent-based modeling
- Simulation starts from the most downstream and proceeds to the most upstream echelon by echelon
- Accommodates different inventory policies
- User-specified transportation times
- Developed in Python

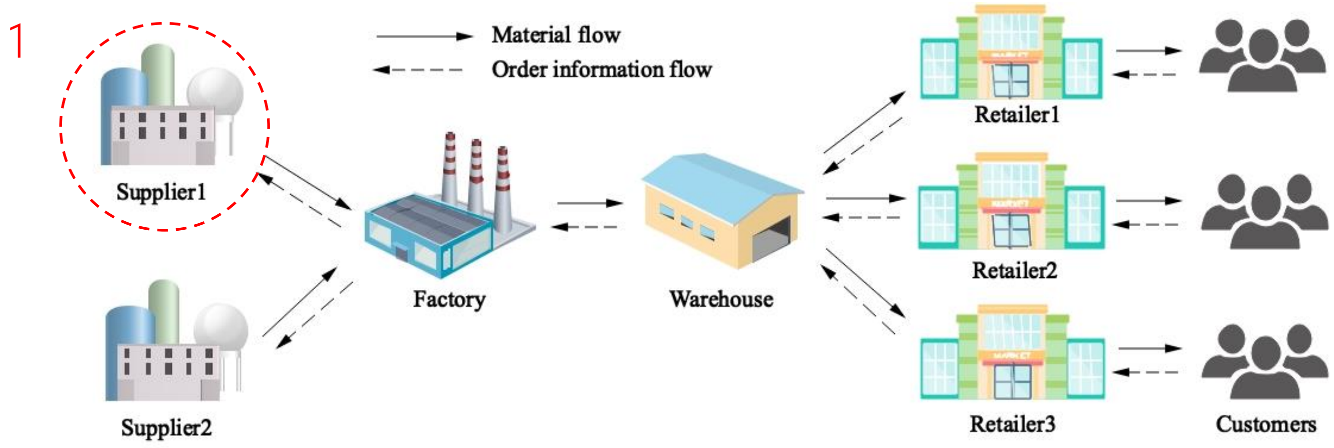


Simulation procedure

- Generate random demand samples
- Sequence of actions of a Retailer:
  - Places an order to Warehouse
  - Receives past orders
  - Satisfies backorders and demand of Customer
  - Updates inventory profiles
- Sequence of actions of a Warehouse:
  - Places an order to Factory
  - Receives past orders
  - Satisfies backorders and orders of Retailers
  - Updates inventory profiles
- ……

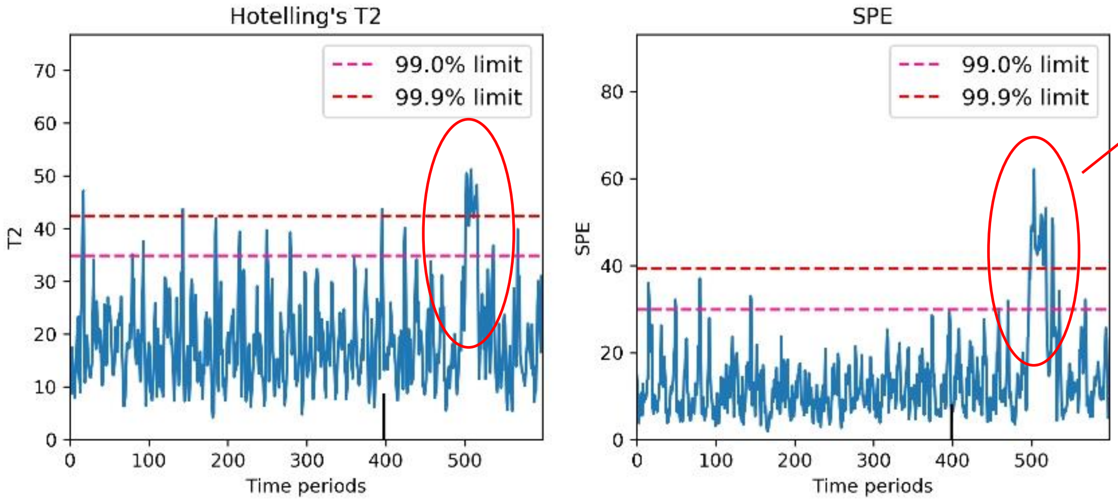
Case study I: A multi-echelon supply chain

Fault: Raw material shortage



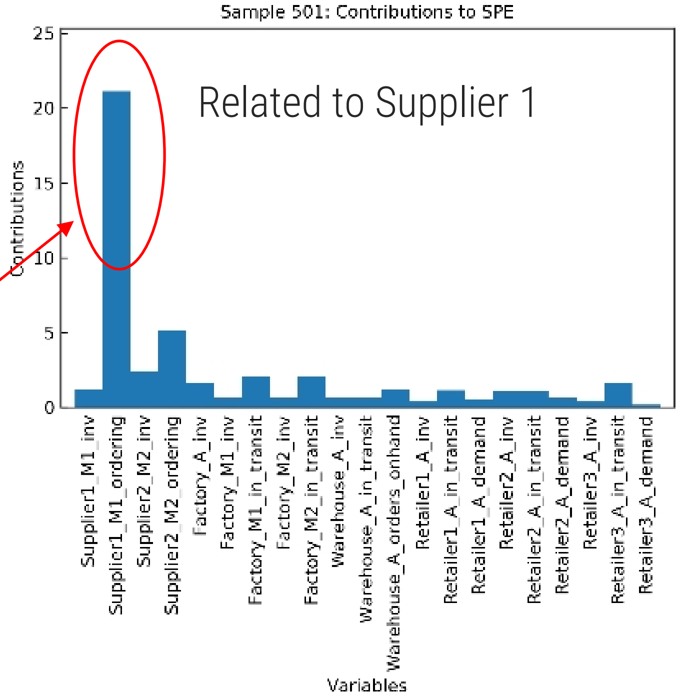
Wang, J., Swartz C.L.E., Corbett, B., and Huang, K. Ind. Eng. Chem. Res., 59(27):12487-12503, 2020.

Fault detection: DPCA monitoring charts



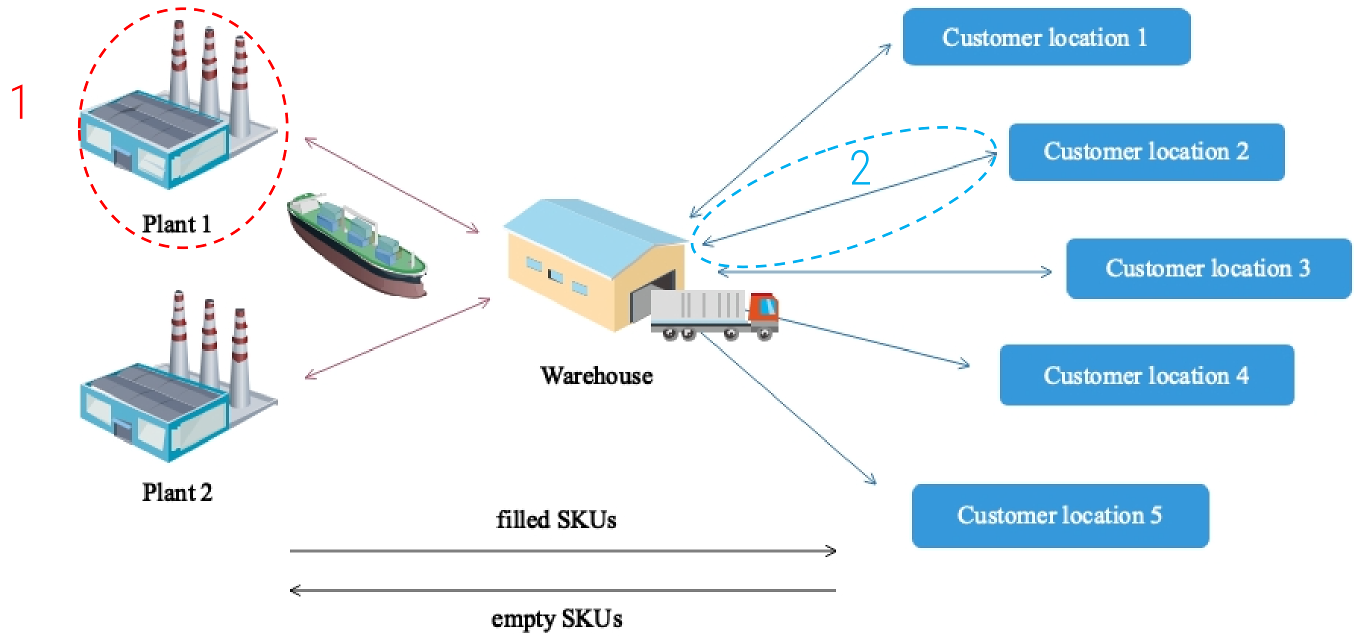
Fault diagnosis:

SPE contributions at the beginning of the stockout



The abnormality is detected soon after the stockout occurs at the supplier, before it affects downstream agents.

Case study II: A packaged liquefied gas supply chain *



Wang, J., Swartz C.L.E., Corbett, B., and Huang, K. Ind. Eng. Chem. Res., 59(27):12487-12503, 2020.

Fault scenarios:

1. Reduced yield – Plant 1
2. Transportation delay

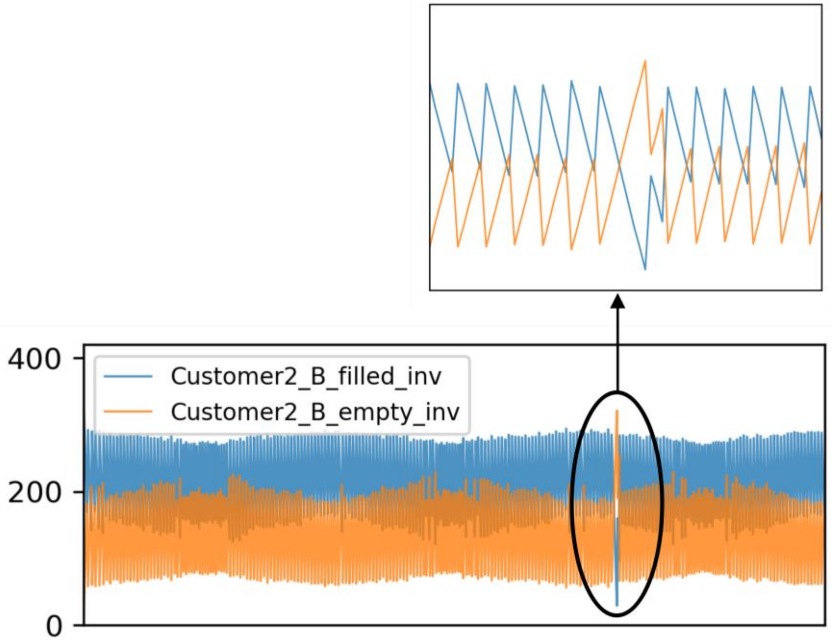
- Flow of filled stock keeping units (SKUs) from upstream to downstream
- Flow of empty SKUs from downstream to upstream
- Demand: multivariate Gaussian, seasonality
- Data for 60 variables: Demand of products A and B (10), inventory levels (24), SKUs in transit and at plants (26)
- NOC data: DPCA using 2 lags →180 variables. 50 PCs explain 95% of variance.

* Misra, S., Kapadi, M., Gudi, R.D., Saxena, D., Ind. Eng. Chem. Res., 58, 7579-7592, 2019.

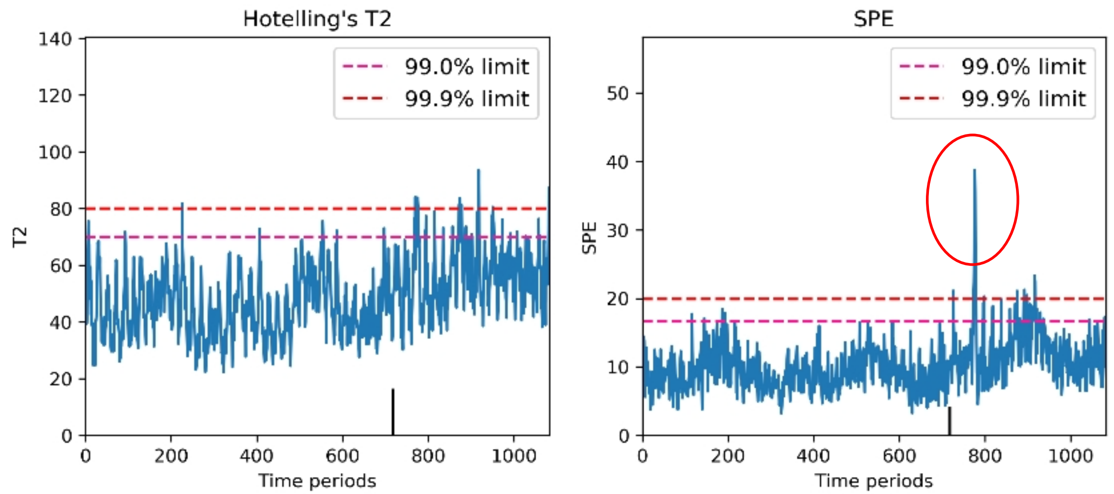
Case study II: A packaged liquefied gas supply chain *

Fault scenario 2

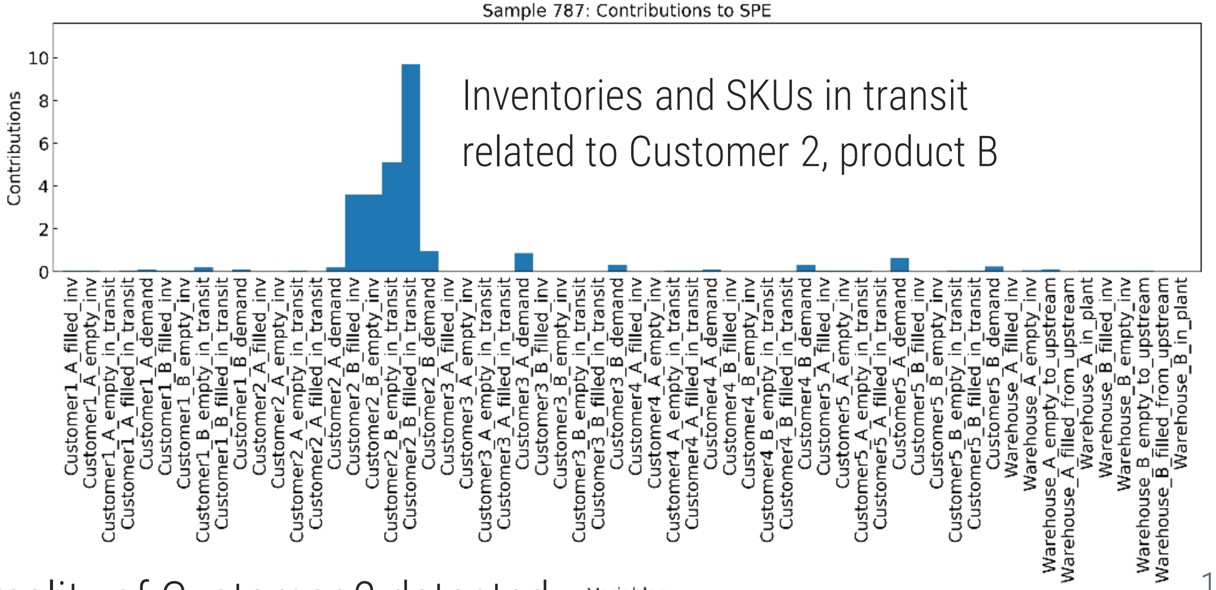
- Seasonal demands
- Transportation delay of product B to Customer 2



Fault detection: DPCA monitoring charts



Fault diagnosis: SPE contributions



Abnormality of Customer 2 detected.

Canonical Variate Analysis (CVA)

- Based on reduced dimension dynamic (state space) model.
- Considered to be more suitable for dynamic systems.
- Literature studies indicate superior performance to PCA for dynamic systems, under various metrics and applications.
- Motivated investigation of CVA for supply chain monitoring.
- Useful literature sources:
  - Negiz, A, Cinar, A (1997). AIChE J., 43(8), 2002-2020.
  - Russell, E, Chiang, LH, Braatz, RD (2000). Data-driven Methods for Fault Detection and Diagnosis in Chemical Processes, Springer-Verlag, London.
  - Jiang, B, Huang, D, Zhu, X, Yang, F, Braatz, RD (2015). J. Process Control, 26, 17-25.

Canonical Variate Analysis

- Consider a dynamic system in state-space form

$$x(t+1) = Ax(t) + Bu(t) + v(t)$$
$$y(t) = Cx(t) + Du(t) + Ev(t) + w(t)$$

State $x(t)$, input $u(t)$, output $y(t)$, disturbances $v(t), w(t)$.

- Construct past & future vectors:

$$p(t) = [y^T(t-1), y^T(t-2), \ldots, y^T(t-l), u^T(t-1), u^T(t-2), \ldots, u^T(t-l)]^T$$
$$f(t) = [y^T(t), y^T(t+1), \ldots, y^T(t+h)]^T$$

- Find α, β to maximize the correlation:

$$\max_{\alpha,\beta} corr(\alpha^T p, \beta^T f) = \frac{\alpha^T \Sigma_{pf} \beta}{\sqrt{\alpha^T \Sigma_{pp} \alpha}\sqrt{\beta^T \Sigma_{ff} \beta}}$$

where

Σ_{pp}, Σ_{ff}: covariance matrices

Σ_{pf}: cross-covariance matrix

- Solution via

$$\Sigma_{pp}^{-1/2} \Sigma_{pf} \Sigma_{ff}^{-1/2} = U \Sigma V^T$$

- Issue: invertible matrices

Canonical Variate Analysis

To address singular matrices:

- Sparse CVA (SCVA) (Witten at al., 2009; Lu et al., 2018)

$$\max_{\alpha,\beta} \alpha^T P^T F \beta$$
$$\text{s. t.} \quad \|\alpha\|_2 \le 1, \|\beta\|_2 \le 1, \|\alpha\|_1 \le c_1, \|\beta\|_1 \le c_2$$

- Problem solved by a penalized matrix decomposition

- Result: Projection matrix J_d

- Canonical states: $x_d(t) = J_d p(t)$

CVA-based fault detection & diagnosis

Monitoring statistics:

- Canonical state space:

$$T_d^2(t) = x_d^T(t)\Sigma_{dd}^{-1}x_d(t) \sim \frac{d(N^2-1)}{N(N-d)}F(d, N-d)$$

where Σ_{dd}: covariance matrix of $x_d(t)$

- Residual space:

$$Q(t) = r^T(t)r(t)$$
where $r(t) = [I - J_d^T(J_d J_d^T)^{-1}J_d]p(t)$

Confidence limit determined by its corresponding percentile of training data.

Canonical Variate Analysis

Variable contributions

- Contribution of input to the canonical state space

$$C_{u_k}^d(t) = \sum_{j=1}^{l} x_d^T(t)\Sigma_{dd}^{-1} u_k(t-j) J_{d,k_j}$$

where k_j is the index of the column of J_d that corresponds to variable $u_k(t-j)$.

- Contribution of input to the residual space

$$C_{u_k}^r(t) = \sum_{j=1}^{l} r^T(t) u_k(t-j) J_{e,k_j}$$

where $J_e = I - J_d^+ J_d$, and k_j is the index of the column of J_e that corresponds to variable $u_k(t-j)$.

- Combined contribution

$$C_{u_k}^{com}(t) = \frac{1}{2}\left[|C_{u_k}^d(t)| + |C_{u_k}^r(t)|\right]$$

Data-driven SCMo Using CVA

A general supply chain system modeled by using the mass balances:

$$I_{t+1}^{a,m} = I_t^{a,m} - \sum_{i \in ADJ(a)+a} Q_t^{a,i,m} + \sum_{j \in ADJ(a)+a} Q_{t-\delta_{j,a}}^{j,a,m}, \qquad \forall a \in A, m \in M, t \in T$$

$$B_{t+1}^{a,m} = B_t^{a,m} - \sum_{i \in ADJ(a)} Q_t^{a,i,m} + \sum_{i \in ADJ(a)} O_t^{i,a,m} + D_t^{a,m}, \qquad \forall a \in A, m \in M, t \in T$$

where

$a \in A$: supply chain agents

$m \in M$: materials

$t \in T$: time periods

$I_t^{a,m}$, $B_t^{a,m}$: inventory, backlog of material m at agent a at period t

$Q_t^{a,i,m}, Q_t^{j,a,m}$: transportation quantities

$O_t^{i,a,m}$: order quantity

$D_t^{a,m}$: customer demand

Data-driven SCMo Using CVA

Variable lifting:

Introduce $\delta_{j,a}$ auxiliary variables, $Q^{j,a,m}_{t,k}$, $k = 1, 2, \dots, \delta_{j,a}$:

$$\begin{bmatrix} Q^{j,a,m}_{t+1,1} \\ Q^{j,a,m}_{t+1,2} \\ \vdots \\ Q^{j,a,m}_{t+1,\delta_{j,a}-1} \\ Q^{j,a,m}_{t+1,\delta_{j,a}} \end{bmatrix} = \begin{bmatrix} Q^{j,a,m}_{t,2} \\ Q^{j,a,m}_{t,3} \\ \vdots \\ Q^{j,a,m}_{t,\delta_{j,a}} \\ Q^{j,a,m}_{t} \end{bmatrix}, \quad \forall t$$

Then,

$$I^{a,m}_{t+1} = I^{a,m}_t - \sum_{i \in ADJ(a)+a} Q^{a,i,m}_t + \sum_{j \in ADJ(a)+a} Q^{j,a,m}_{t,1}, \qquad \forall a, m, t$$

$$B^{a,m}_{t+1} = B^{a,m}_t - \sum_{i \in ADJ(a)} Q^{a,i,m}_t + \sum_{i \in ADJ(a)} O^{i,a,m}_t + D^{a,m}_t, \qquad \forall a, m, t$$

$$Q^{j,a,m}_{t+1,k} = Q^{j,a,m}_{t,k+1}, \qquad \forall a, m, t, k = 1, 2, \dots, \delta_{j,a} - 1$$

$$Q^{j,a,m}_{t+1,\delta_{j,a}} = Q^{j,a,m}_t, \qquad \forall a, m, t$$

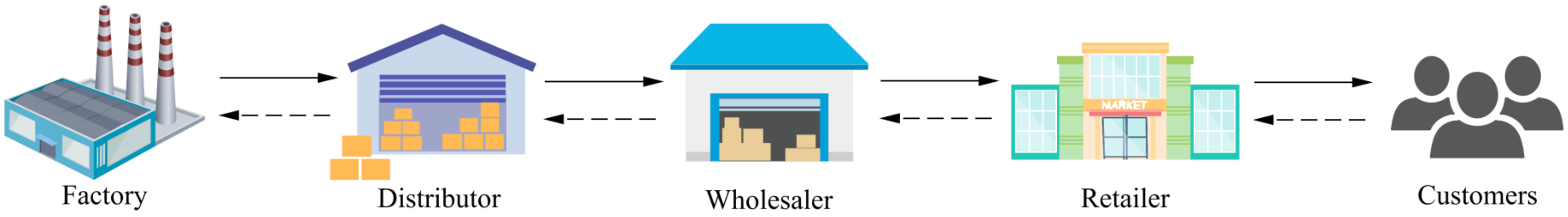
Data-driven SCMo Using CVA

Supply chain state space model takes the form:

$$x(t+1) = Ax(t) + Bu(t) + v(t)$$
$$y(t) = Cx(t)$$

$$x(t) = \left[\left(I_t^{a,m} \forall a, m \right), \left(B_t^{a,m} \forall a, m \right), \left(Q_{t,k}^{j,a,m} \forall a, j, m, k \right) \right]^T$$
$$u(t) = \left[\left(Q_t^{a,i,m} \forall a, i, m \right), \left(O_t^{i,a,m} \forall a, i, m \right) \right]^T$$
$$v(t) = \left[\left(D_t^{a,m} \forall a, m \right) \right]^T$$
$$y(t) = \left[\left(I_t^{a,m} \forall a, m \right), \left(B_t^{a,m} \forall a, m \right) \right]^T$$

Case study I: The beer distribution game



Wang, J., Swartz C.L.E., Huang, K. (2023). Comp. Chem. Eng., in press.

Demand pattern

- Normal distribution
- Seasonal autoregressive integrated moving average (SARIMA)

$$\phi_p(B)\Phi_P(B^s)\nabla^d\nabla_s^D x_t = \theta_q(B)\Theta_Q(B^s)a_t$$

Inventory policies

- (S-1, S)/1-1 policy. S – target inventory.
- (R, S) policy. R – review period, S – target inventory.

Supply chain variables (17)

- Inputs (9): quantities of production, shipment, order, sale, demand
- Outputs (8): stock on hand, backlog

Fault scenarios:

1. Transportation delay: Wholesaler, Retailer
2. Transportation delay: Distributor, Wholesaler
3. Transportation delay: Factory, Distributor
4. Reduced yield: Factory
5. Customer demand: an increase
6. 1 & 2; 3 & 4

Performance metrics:

1. Dimensionality reduction
2. False alarm rate (FAR)
3. Missed detection rate (MDR)
4. Detection delay

Case study I: The beer distribution game

SCVA hyperparameter tuning

- Training set comprises SC data collected over 1000 time periods
- Time lags (*l*=*h*=2) determined from autocorrelation plot
- For each candidate hyperparameter pair (d, c):
  - CVA model is fitted to different subsets constructed by partitioning the training set.
  - Average mean squared error (MSE) is calculated

recalling that

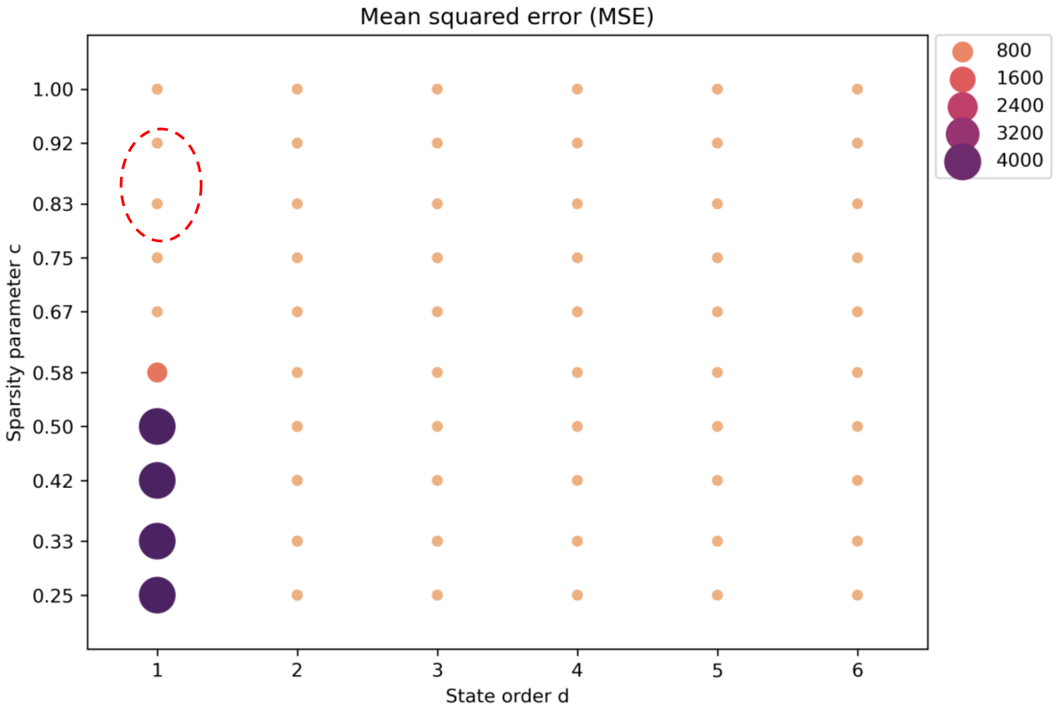
d = state order; c1, c2 = sparsity parameters

where $c_1 = c\sqrt{n_p}, c_2 = c\sqrt{n_f}$

34 SC variables reduced to 1 canonical state

- Demand ~ normal distribution
- 1-1 inventory policy

Metric: average MSE



Wang, J., Swartz C.L.E., Huang, K. (2023). Comp. Chem. Eng., in press.

Selected hyperparameters:

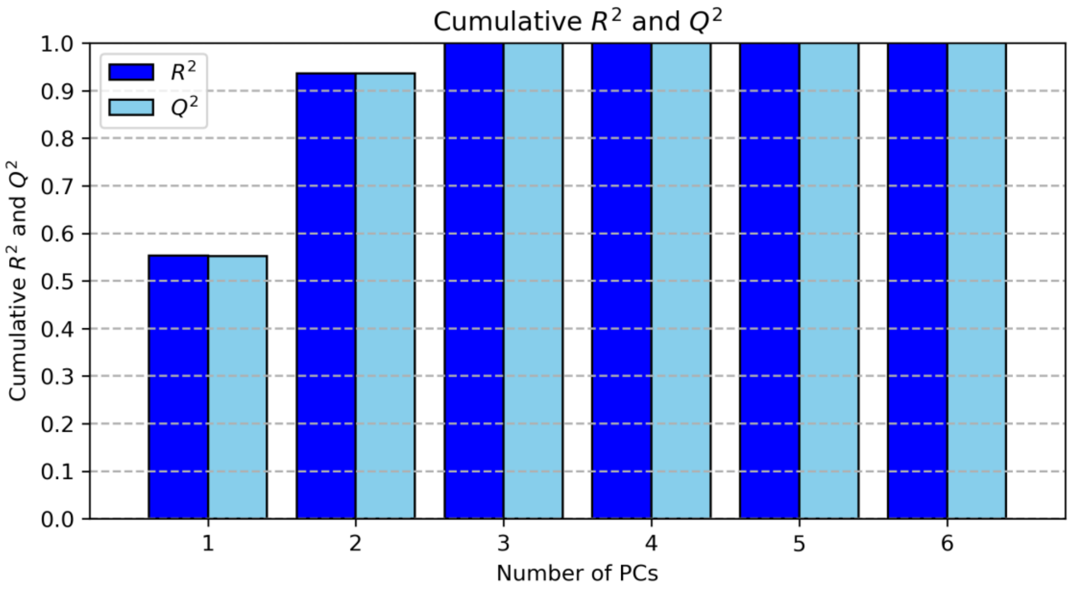
- State order d = 1
- sparsity parameter c = 0.8

Case study I: The beer distribution game

DPCA hyperparameter tuning

Metrics:

- R^2: explained variance of training set
- Q^2: explained variance of validation set



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Selected number of PCs: 2

FAR – type I error rate, false positive rate:

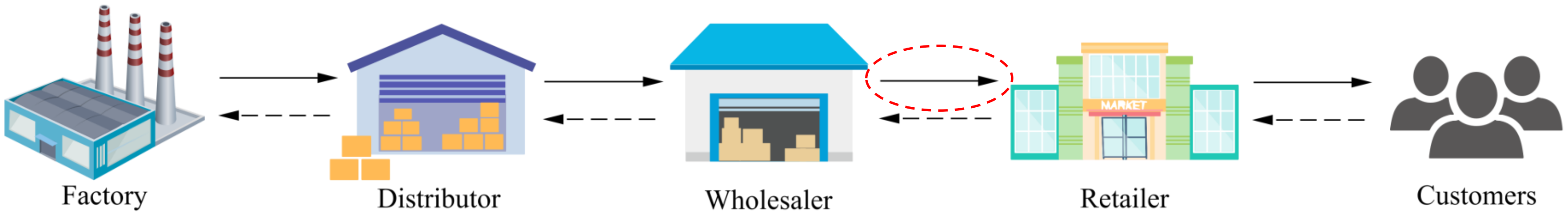
ratio of false alarms relative to the total samples.

Table: average false alarm rate

Demand	Policy	Lag l, h	SCVA				DPCA			
			N_{CS}	T_d^2	Q	$S_{overall}$	N_{PC}	T^2	SPE	$S_{overall}$
Normal	1-1	2	1	0.013	0.013	0.026	2	0.014	0.01	0.024
Normal	(R, S)	4	4	0.013	0.013	0.026	6	0.013	0.012	0.025
SARIMA	1-1	8	3	0.036	0.036	0.069	5	0.068	0.01	0.076
SARIMA	(R, S)	11	3	0.029	0.053	0.078	8	0.093	0.015	0.106

- SCVA achieves comparable performance to DPCA in terms of FAR in a lower dimensional latent space.
- The level of FAR can be case-dependent.

Case study I: The beer distribution game



Wang, J., Swartz C.L.E., Huang, K. (2023). Comp. Chem. Eng., in press.

Fault scenario:

- Transportation delay: Wholesaler, Retailer
- Retailer experiences a longer transportation delay (4 periods) for its orders. The normal delay is 2 periods.

Observations

- Q-statistic exceeds its 99% limit, indicating suspected presence of fault.
- Largest contributions associated with retailer inventory and backorders

Case study I: The beer distribution game

Missed detection rate (MDR)

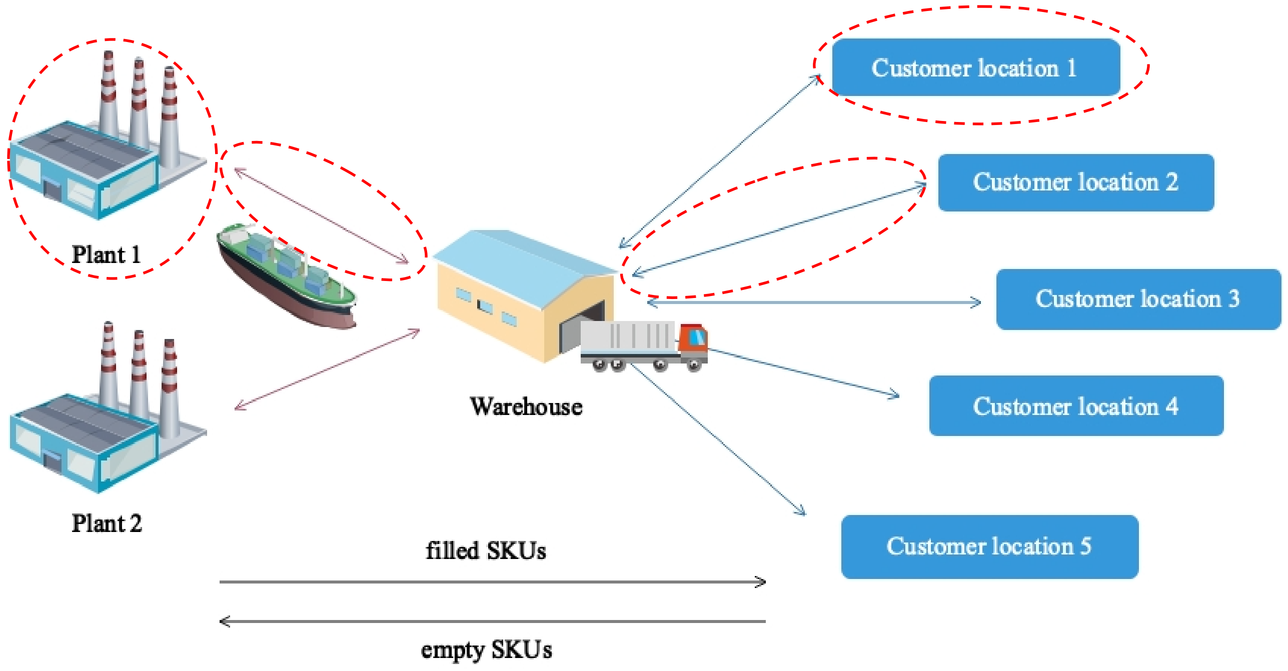
- Type II error rate, false negative rate
- The ratio of undetected faulty samples relative to the total number of faulty samples under a specific fault.

Table: missed detection rate

Demand	Policy	Fault	SCVA			DPCA		
			T_d^2	Q	$S_{overall}$	T^2	SPE	$S_{overall}$
Normal	1-1	1	0.96	0	0	0.95	0	0
Normal	1-1	2	0.94	0	0	0.94	0	0
Normal	1-1	3	0.94	0	0	0.94	0	0
Normal	(R, S)	1	0.92	0.05	0.05	0.97	0	0
Normal	(R, S)	2	0.97	0.02	0.02	0.97	0	0
Normal	(R, S)	3	0.94	0.02	0.02	0.95	0	0
SARIMA	1-1	1	0.81	0.02	0.01	0.73	0.03	0.02
SARIMA	1-1	2	0.8	0.02	0.01	0.74	0.03	0.02
SARIMA	1-1	3	0.8	0.02	0.01	0.74	0.03	0.02
SARIMA	(R, S)	1	0.82	0.06	0.05	0.75	0	0
SARIMA	(R, S)	2	0.79	0.07	0.07	0.7	0	0
SARIMA	(R, S)	3	0.87	0.05	0.05	0.75	0	0

- Q in SCVA and SPE in DPCA are more reliable for detecting faults than T_d^2 and T^2.
- Consistent with Russel et al. (2000) in application to Tennessee Eastman problem
- SCVA achieves comparable performance to DPCA in terms of missed detection rate.

Case study II: A packaged liquefied gas supply chain *



Wang, J., Swartz C.L.E., Corbett, B., and Huang, K. Ind. Eng. Chem. Res., 59(27):12487-12503, 2020.

Supply chain variables (58)

- Inputs (34): shipment quantities
- Outputs (24): inventories

Demand patterns:

- Cross-correlation

  Multivariate Gaussian distribution

- Autocorrelation

  Vector autoregressive moving average (VARMA):

$$y_t = \sum_{i=1}^{p} A_i y_{t-i} + \varepsilon_t + \sum_{j=1}^{q} M_j \varepsilon_{t-j}$$

Fault scenarios:

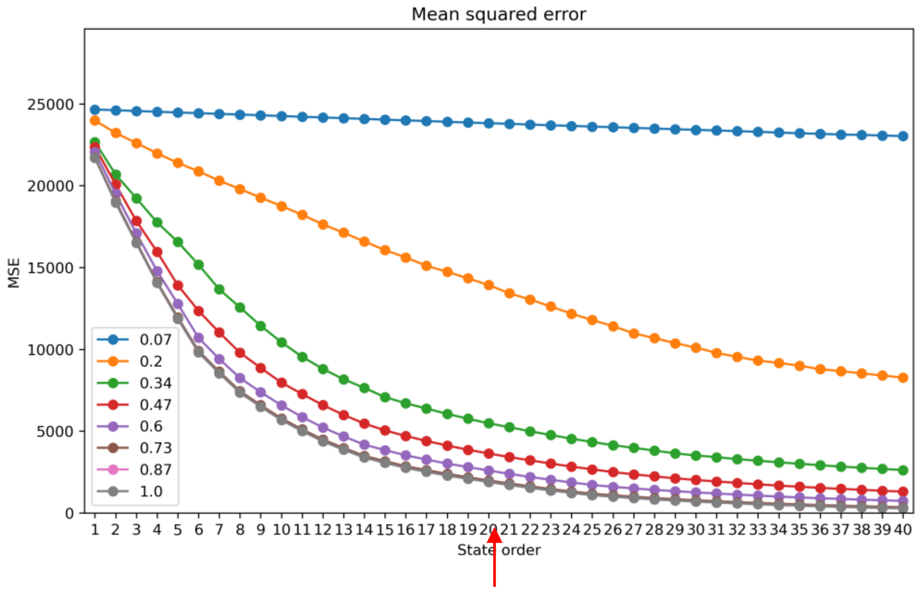
1. Transportation delay: Warehouse, Customer
2. Transportation delay: Plant, Warehouse
3. Plant refilling delay
4. Change of Customer demand
5. 1&2; 1&4; 2&3

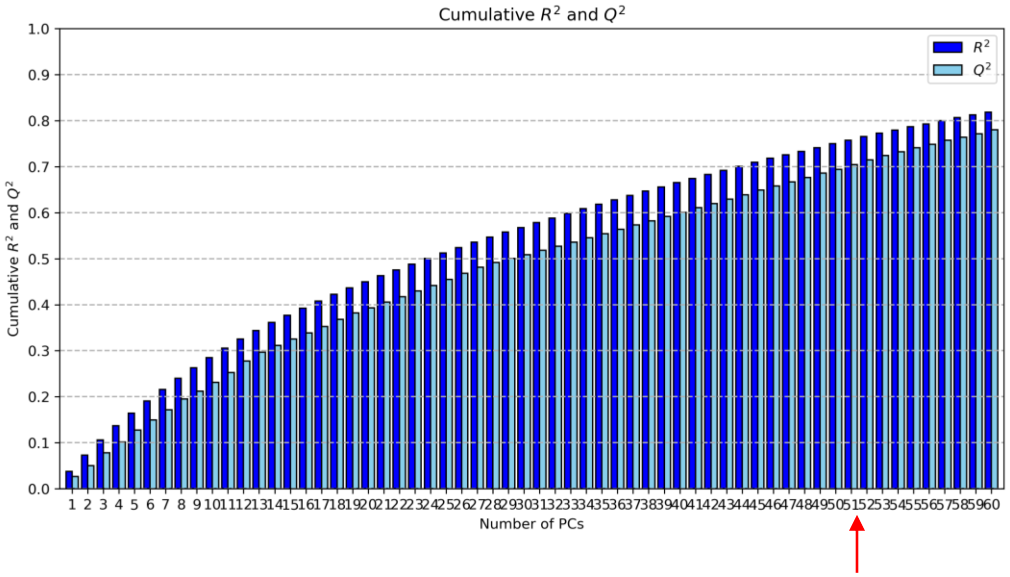
* Misra, S., Kapadi, M., Gudi, R.D., Saxena, D., Ind. Eng. Chem. Res., 58, 7579-7592, 2019.

Case study II: A packaged liquefied gas supply chain

Hyperparameter tuning

- Demand ~ multivariate Gaussian distribution
- 58 variables x lag order 8
- Lag order via autocorrelation plot
- 2000 training samples





- SCVA: 20 canonical states for a low MSE, with sparsity c ∈ [0.7, 1]
- DPCA: 51PCs, with $R^2 \approx 76\%$, $Q^2 \approx 70\%$

SCVA uses significantly fewer latent variables; 464 variables reduced to 20 canonical states.

Case study II: A packaged liquefied gas supply chain

Table: average false alarm rate

Demand	Lag l, h	SCVA				DPCA			
		N_{CS}	T_d^2	Q	$S_{overall}$	N_{PC}	T^2	SPE	$S_{overall}$
Gaussian	8	20	0.011	0.011	0.022	51	0.012	0.01	0.021
VARMA	8	30	0.001	0.041	0.041	57	0.006	0.065	0.069

- More canonical states and latent variables needed under autocorrelated demand
- SCVA achieves comparable performance to DPCA in terms of false alarm rate.

Case study II: A packaged liquefied gas supply chain

Table: missed detection rate

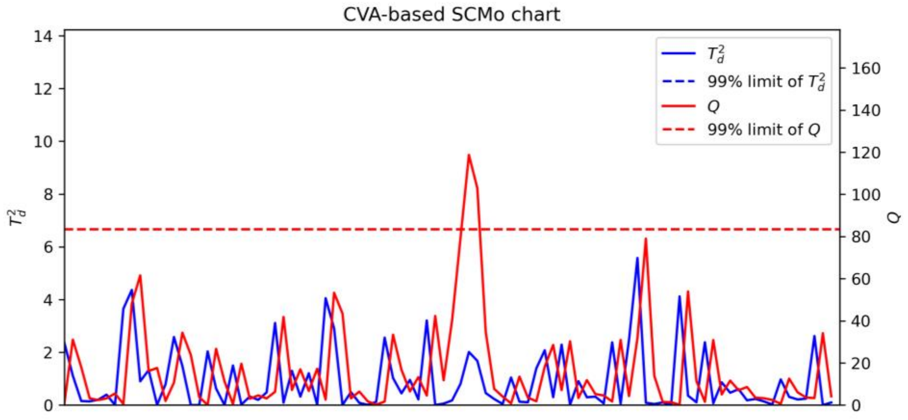
Demand	Fault	SCVA			DPCA		
		T_d^2	Q	$S_{overall}$	T^2	SPE	$S_{overall}$
Gaussian	1	0.71	0	0	0.87	0	0
Gaussian	2	0.92	0	0	0.96	0	0
Gaussian	3	0.91	0.04	0.03	0.96	0	0
Gaussian	4	0.84	0	0	0.44	0	0
Gaussian	5	0.63	0.02	0.02	0.71	0	0
Gaussian	6	0.78	0.13	0.12	0.85	0.02	0.01
Gaussian	7	0.92	0.04	0.03	0.96	0	0
VARMA	1	1	0	0	0.88	0	0
VARMA	2	0.95	0.01	0.01	0.88	0	0
VARMA	3	0.94	0.1	0.1	0.92	0	0
VARMA	4	0.9	0.06	0.06	0.19	0.07	0.06
VARMA	5	0.97	0.06	0.06	0.72	0.01	0.01
VARMA	6	0.99	0	0	0.94	0	0
VARMA	7	0.99	0.05	0.05	0.92	0	0

- Both SCMo models rely on the statistic in the residual space.
- SCVA achieves comparable performance to DPCA in terms of missed detection rate.

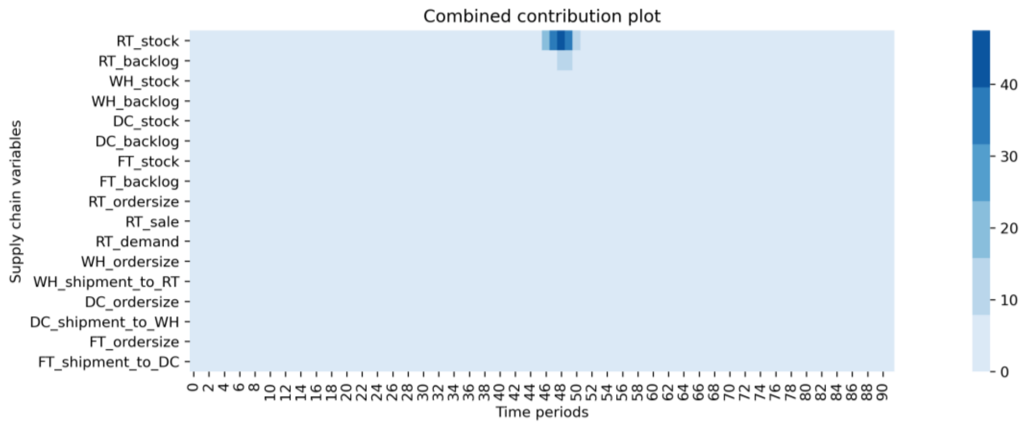
Fault Impact Prediction

Current literature

✓ fault detection



✓ fault diagnosis/identification



- Studies on CVA-based monitoring are focused on detecting and diagnosing a fault in the observation p(t).
- The ability of CVA in modeling the relationship between p(t) and f(t) has not been fully explored and utilized.

❑ fault impact prediction

- Proposed CVA-based method of predicting the impact of a fault, i.e., identifying potentially impacted variables.

Fault Impact Prediction

The optimal estimate of the future vector based on CVA (Larimore, 1990; Lu et al, 2018):

$$\hat{f}(t) = \Sigma_{fd}\Sigma_{dd}^{-1}x_d(t) = \Sigma_{fd}\Sigma_{dd}^{-1}J_d p(t) = J_{fp}p(t)$$

where Σ_{fd} is the cross-covariance matrix between $f(t)$ and $x_d(t)$.

Recall:

$p(t) = [y^T(t-1), y^T(t-2), \ldots, y^T(t-l), u^T(t-1), u^T(t-2), \ldots, u^T(t-l)]^T$

$f(t) = [y^T(t), y^T(t+1), \ldots, y^T(t+h)]^T$

An input variable u_k over the l time lags:

$$u_k^l(t) = [u_k(t-1), u_k(t-2), \ldots, u_k(t-l)]^T$$

An output variable y_i and predicted $\hat{y}_i^h(t)$ over the h future periods:

$$y_i^h(t) = [y_i(t), y_i(t+1), \ldots, y_i(t+h-1)]^T$$

$$\hat{y}_i^h(t) = [\hat{y}_i(t), \hat{y}_i(t+1), \ldots, \hat{y}_i(t+h-1)]^T$$

A disturbance in $u_k^l(t)$, $\Delta u_k^l(t)$, causes a change in $\hat{y}_i^h(t)$:

$$\Delta\hat{y}_i(t+a) = \sum_{j=1}^{l} J_{fp}(r_{i,a}, c_{k,j}) \cdot \Delta u_k(t-j), \quad \forall a = 0, 1, \ldots, h-1$$

Define a fault impact indicator by assuming $\Delta u_k(t-j) = \Delta u_k^0$, $j = 1, 2, \ldots, l$:

$$FI(y_i, u_k) = \frac{\|\Delta\hat{y}_i^h(t)\|_2}{\|\Delta u_k^l(t)\|_2} = \left[\sum_{a=0}^{h-1}\left[\sum_{j=1}^{l} J_{fp}(r_{i,a}, c_{k,j})\right]^2\right]^{\frac{1}{2}}$$

Large $FI(y_i, u_k)$ indicates that y_i is likely to be affected by the disturbance in u_k.

Fault Impact Prediction

1. Estimate the fault impact matrix from the NOC training data:

$$FI = [[FI(y_i, y_g)], [FI(y_i, u_k)]]$$

2. When a fault is detected, calculate and normalize the combined contribution vector:

$$\overline{C^{com}}(t) = \frac{C^{com}(t)}{\|C^{com}(t)\|_1} = [\overline{C^{com}_{y_1}}(t), \ldots, \overline{C^{com}_{y_{m_y}}}(t), \overline{C^{com}_{u_1}}(t), \ldots, \overline{C^{com}_{u_{m_u}}}(t)]^T$$

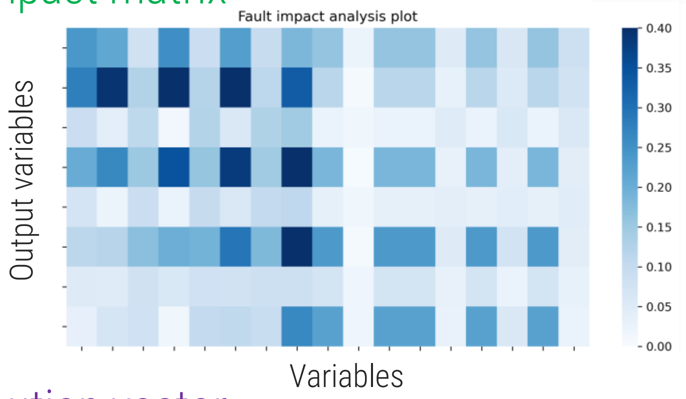
Components of the vector can be interpreted as the probability of the corresponding variables being fault-related.

3. Calculate the expected relative variation of output variables:

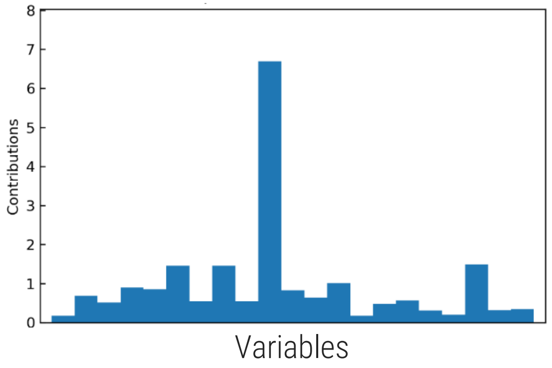
$$FP(t) = FI \cdot \overline{C^{com}}(t)$$

A large component of the vector FP(t) indicates that the corresponding variable is likely to be impacted by the fault.

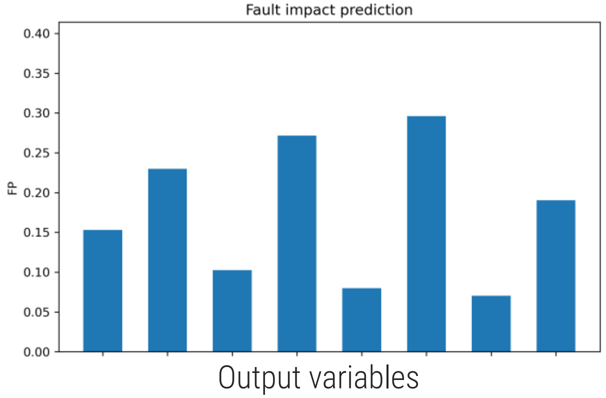
fault impact matrix



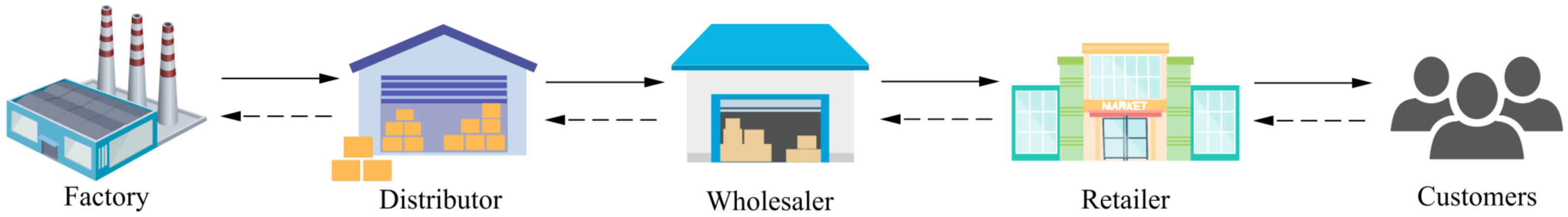
contribution vector



expected relative variation



Fault Impact Prediction



Wang, J., Swartz C.L.E., Huang, K. (2023). Comp. Chem. Eng., in press.

- Inventory policy: 1-1 policy
- Demand ~ normal distribution
- Transportation delays: 4 time periods

SCVA model:

- 17 supply chain variables:

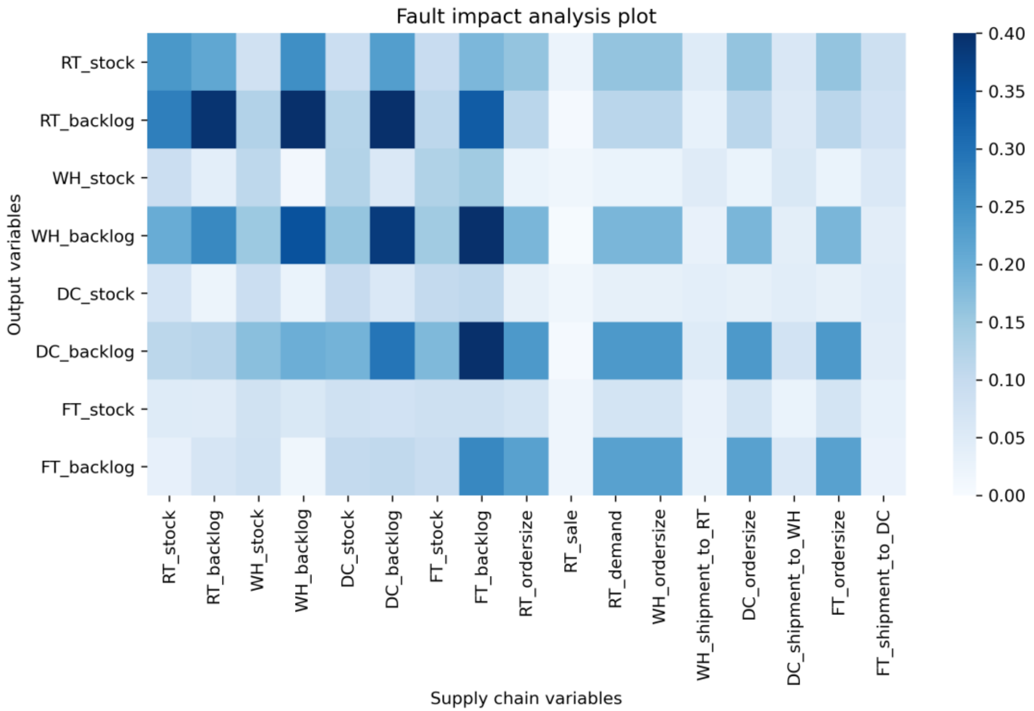
  Inputs (9): quantities of production, shipment, order, sale, demand

  Outputs (8): stock on hand, backlog
- Lag orders l = h = 4
- State order d = 3, sparsity c = 0.8

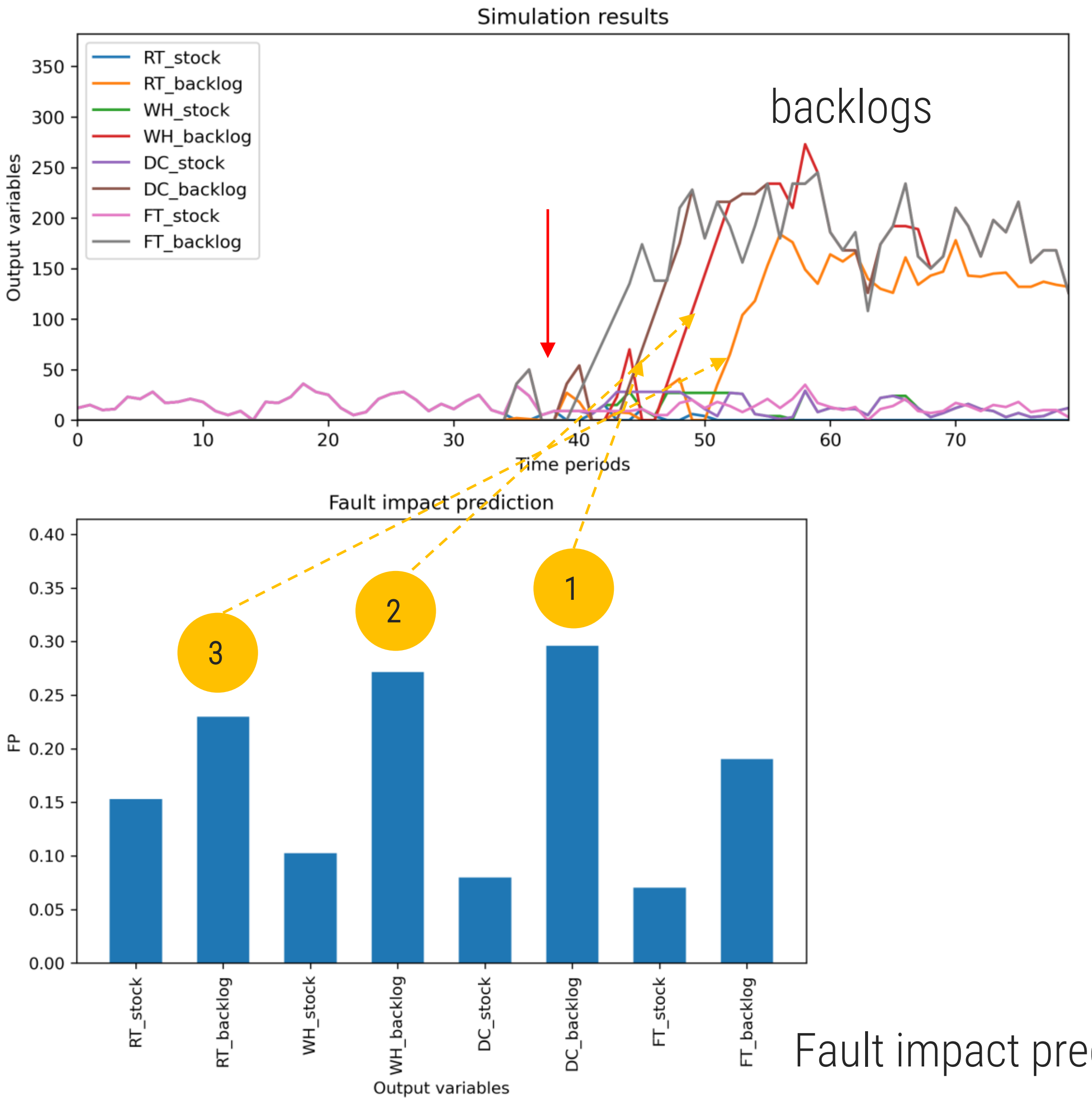
Fault scenario:

- Production of factory shuts down for 5 time periods
- Impact - stockout: factory → distributor → wholesaler → retailer

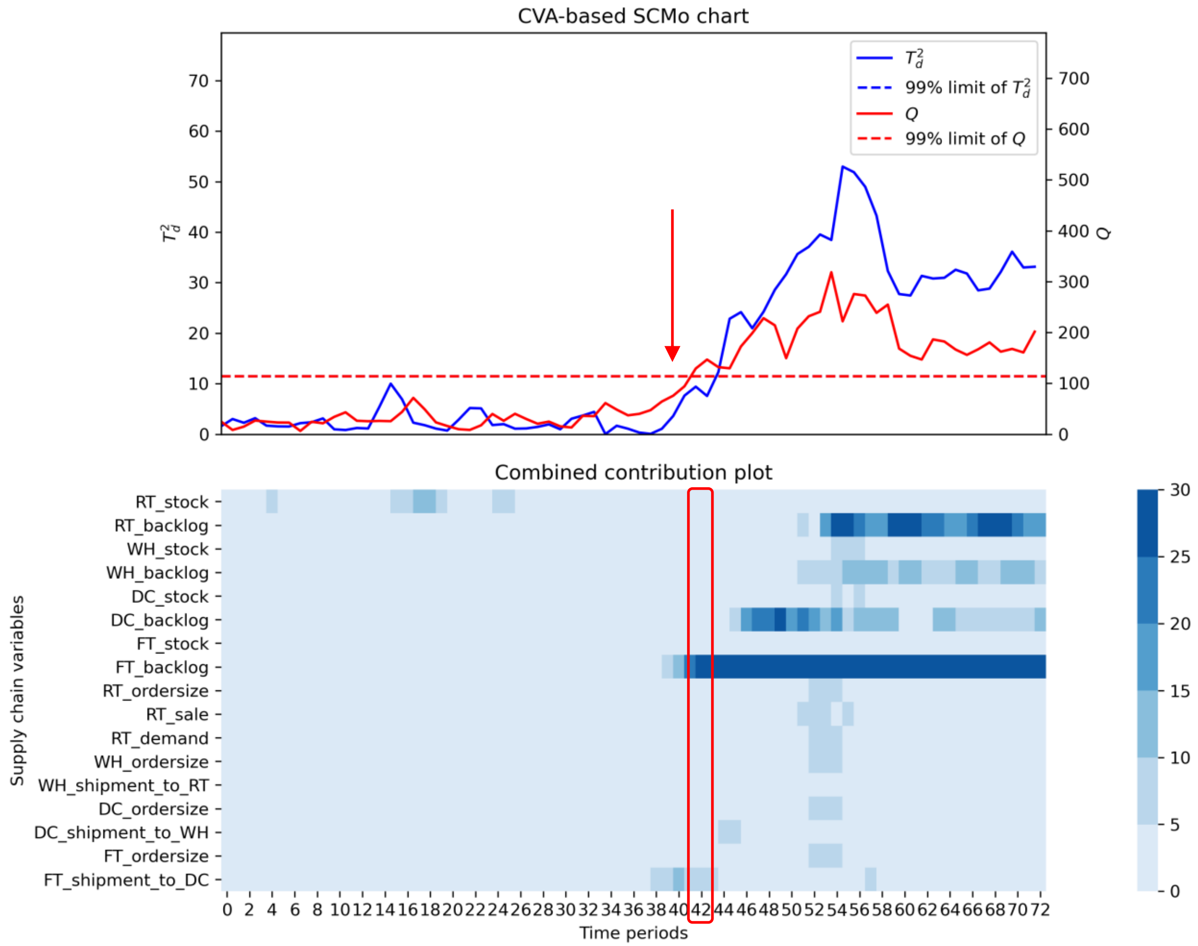
Fault impact indicator matrix from NOC data



Fault Impact Prediction



Fault detection & diagnosis



Fault impact prediction vector ⇐ Contribution vector

Conclusions

- Multivariate statistical methods are shown to be promising for supply chain monitoring.
- Abnormal behavior of the supply chain, e.g., transportation delay, low production rate, and supply shortage, can be successfully detected by PCA and CVA.
- Contribution plots can help interpret the abnormality and identify the fault-related variables.
- CVA can achieve comparable performance in a lower dimensional latent space.
- The proposed fault impact prediction method is effective.

Future work

- Application to real-world supply chain systems.
- Identify limitations of methodology, and refine.