Tensor Mixed-Effects Model, With Application to Nanomanufacturing

--- Engineering-Driven Data Analytics for Advanced Manufacturing

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INTRODUCTION

The **objective** of this research is to develop engineering-driven data analytics methodologies for nanomanufacturing through systematic and deep integration of data analytics, optimization and manufacturing domain knowledge.

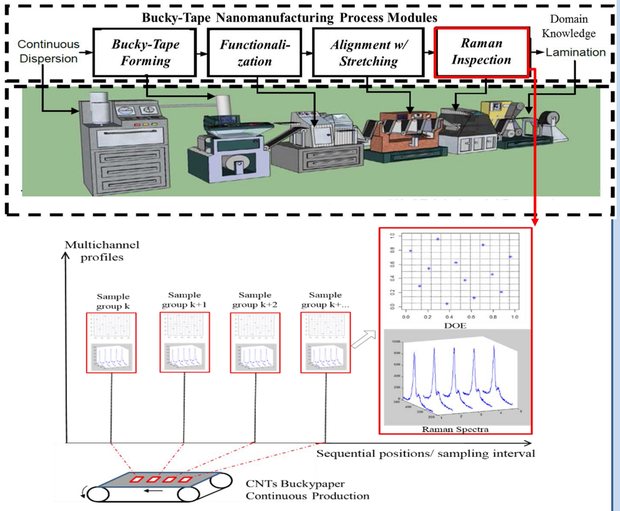


Fig. 1 Nanomanufacturing & Data Collection

CHALLENGES

- **Feature Challenge**: consistency, uniformity, defects
- **Noise Challenge**: Signal dependent noise
- **Data Challenge**: 600+ signals per m, 1000+ shift/intensities per spectrum
- **Correlation Challenge**: Spatial-temporal correlation

METHODOLOGY

Tensor Mixed-Effects (TME) Model

- Separate fixed effects & random effects
- Handle the multi-dimensional arrays (tensors)
- Explore the correlations in different dimensions

Fixed Effects | Random Effects | Noise

$$\mathcal{Y}_i = \mathcal{F} \times_1 \boldsymbol{A}_i^{(1)} \times_2 \boldsymbol{A}_i^{(2)} \times_3 \boldsymbol{A}_i^{(3)} + \mathcal{R}_i \times_1 \boldsymbol{B}_i^{(1)} \times_2 \boldsymbol{B}_i^{(2)} \times_3 \boldsymbol{B}_i^{(3)} + \mathcal{E}_i \quad (1)$$

Fixed effects core tensor | Fixed effects design matrices | Random effects core tensor | Random effects design matrices | Noise tensor

$$\mathcal{Y}_i = \mathcal{F} \times_1 \boldsymbol{A}_i^{(1)} \times_2 \boldsymbol{A}_i^{(2)} \times_3 \boldsymbol{A}_i^{(3)} + \mathcal{R}_i \times_1 \boldsymbol{B}_i^{(1)} \times_2 \boldsymbol{B}_i^{(2)} \times_3 \boldsymbol{B}_i^{(3)} + \mathcal{E}_i$$

J, K, L | P_1, Q_1, R_1 | P_2, Q_2, R_2 | J, K, L

$$\mathcal{R}_i \sim \boldsymbol{N}_{P_2,Q_2,R_2}(\mathcal{O}; \boldsymbol{\Sigma}_r, \boldsymbol{\Psi}_r, \boldsymbol{\Omega}_r) \qquad \mathcal{E}_i \sim \boldsymbol{N}_{J,K,L}(\mathcal{O}; \boldsymbol{\Sigma}_\varepsilon, \boldsymbol{\Psi}_\varepsilon, \boldsymbol{\Omega}_\varepsilon)$$

Contribution: A novel tensor mixed-effects (TME) model was developed to analyze massive high-dimensional data with complex correlation structure.

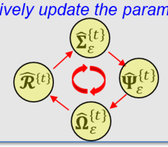
- We also investigate the properties of the TME model, **existence and identifiability** of parameter estimation.
- Numerical analysis demonstrates the **efficiency and accuracy** of the parameter estimation.
- **Convergence and asymptotic properties** are discussed.

ALGORITHM

Step 1: Initialization
High-order orthogonal iteration (HOOI)
Initialize $\hat{\mathcal{F}}^{\{0\}}$, basis matrices and $\hat{\boldsymbol{\Sigma}}_i^{\{0\}}, \hat{\boldsymbol{\Psi}}_i^{\{0\}}, \hat{\boldsymbol{\Omega}}_i^{\{0\}}$

Step 2: First flip-flop algorithm
Iteratively update the parameters

Step 3: Second flip-flop algorithm
Iteratively update the parameters



Complexity

$\mathcal{O}(J^3P_1 + JP_1^4 + P_1^6)$
(Elden and Savas 2009)

J *is dim. of* $\mathcal{Y}_i$
P_1 *is dim. of* $\mathcal{F}$

$\mathcal{O}(NJ^5 + NP_1^9 + NJ^3P_1^3)$

N *is sample size*

$\mathcal{O}(NJ^5)$

Computational complexity of TME is much smaller than the Vectorized LME model.

COMPARISON

Tensor Fixed Effects (TFE) model: $\mathcal{Y}_i = \mathcal{F} \times_1 \boldsymbol{A}_i^{(1)} \times_2 \boldsymbol{A}_i^{(2)} \times_3 \boldsymbol{A}_i^{(3)} + \mathcal{E}_i$

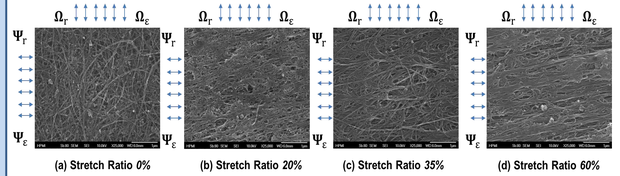
Vectorized Linear Mixed Effects: $\boldsymbol{y}_i = \boldsymbol{X}_i\boldsymbol{\beta} + \boldsymbol{Z}_i\boldsymbol{b}_i + \boldsymbol{\varepsilon}_i$

	Proposed TME	Benchmark 1 (TFE)	Benchmark 2 (vLME)
Tensor Structure	Yes	Yes	No
Random Effects	Yes	No	Yes
Complexity	Low	Low	High
Correlation in Diff. Dim.	Yes	Yes	No

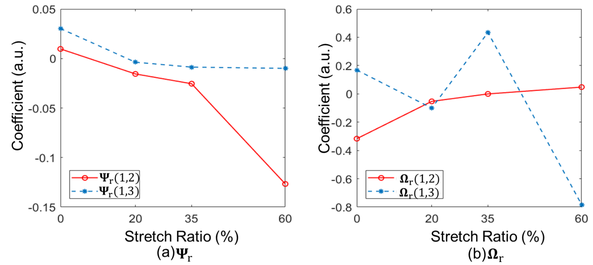
TME model outperforms the benchmark methods.

CASE STUDY

Application to quantifying the degree of alignment in Nanomanufacturing



(a) Stretch Ratio *0%* (b) Stretch Ratio *20%* (c) Stretch Ratio *35%* (d) Stretch Ratio *60%*



REFERENCE

Yue, X., et al. (2019) "Tensor Mixed Effects Model with Applications in Nanomanufacturing Inspection", Technometrics. (won the 2017 INFORMS Data Mining Best Paper Finalist Award)

BIBLIOGRAPHY

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(Open to Collaboration)