Opportunities in tensorial data analytics for chemical and biological manufacturing processes

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- Analysis methods presented and future potential and research scope discussed.

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Existing approaches

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- Average over batches, or time for video, down to an order two tensor (matrix), then continue with PCA, PLS etc. . .
- Can you summarise a film (fourth order tensor, what are the orders?) by averaging all of the frames then converting to greyscale?

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- Can you summarise a film (fourth order tensor, what are the orders?) by averaging all of the frames then converting to greyscale?
- Not very well.
- Can anyone think of a fifth-order tensor?

Second order tensors

Second order tensors

$$\underbrace{\begin{bmatrix} T_1 & V_1 & C_{a_1} & F_{N_1} \\ \vdots & \vdots & \vdots & \vdots \\ T_1 & V_n & C_{a_n} & F_{N_n} \end{bmatrix}}_{\text{single batch process data}}$$

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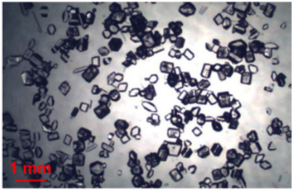

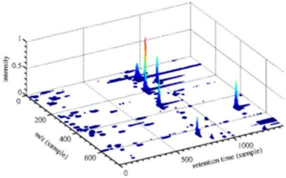

LEFT: grey-scale stereomicroscope image of product crystals with nucleation induced by coaxial mixing. **RIGHT:** Liquid-Chromatography / Mass Spectroscopy analysis has become cheaper and more reliable for online use.

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- Traditional color images for humans however scope for the inclusion of x-rays, infra-red.

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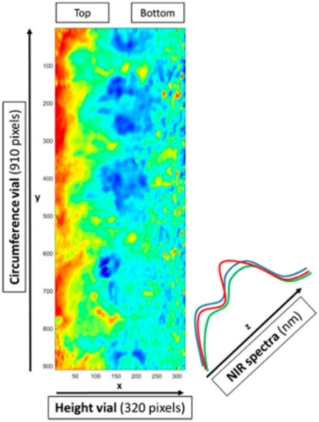

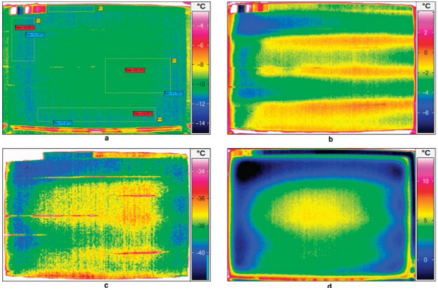

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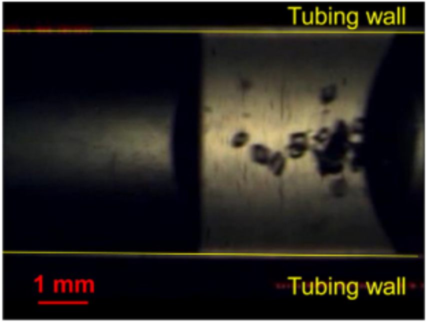

E.g. a spectral video stream of crystal product exiting a tubular crystalliser.

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- **Non-destructive, low-cost, user-friendly.**

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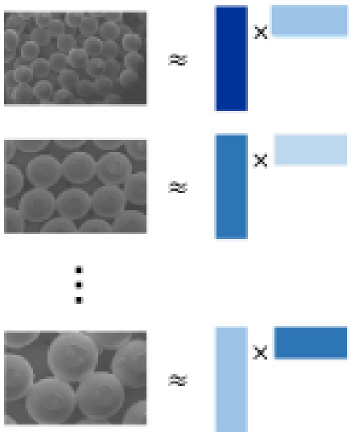

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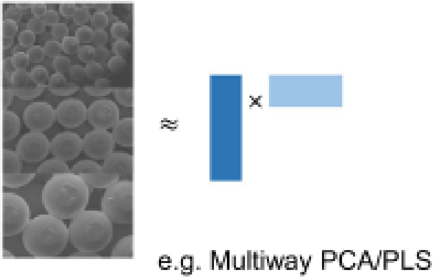

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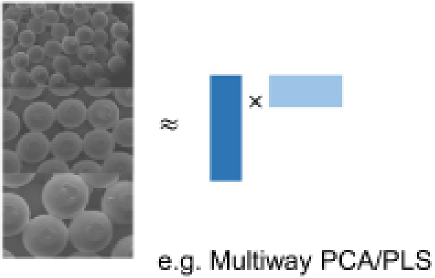

This is extensively used and is called the **multiway method**

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Third approach: Average higher orders to reduce to a second order tensor.

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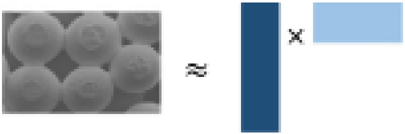

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- Constructed model is often difficult to interpret.

CP decomposition

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Kronecker Product ($\otimes$):

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A sum of these approximations can result in the reconstruction of a full tensor. Generally for a d^{th} order tensor $\mathcal{A} \in \mathbb{R}^{m_1 \times \ldots \times m_d}$ with k components (modes).

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$$\min_{\lambda_k, \mathbf{u}_k^i} \left\| \mathcal{A} - \sum_{k=1}^{K} \lambda_k \mathbf{u}_k^1 \otimes \mathbf{u}_k^2 \otimes \ldots \otimes \mathbf{u}_k^d \right\|_F$$

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- Personally I think stochastic optimisation has huge scope here, not mentioned in review.

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Decomposes a tensor $\mathcal{A}$ into a smaller tensor $\mathcal{T}$ and a series of matrices which reduce the dimension of each tensor-order. For a third-order tensor $\mathcal{A} \in \mathbb{R}^{m_1 \times m_2 \times m_3}$:

$$\tilde{\mathcal{A}} = \mathcal{T} \times_1 \mathbf{U}^1 \times_2 \mathbf{U}^2 \times_3 \mathbf{U}^3$$

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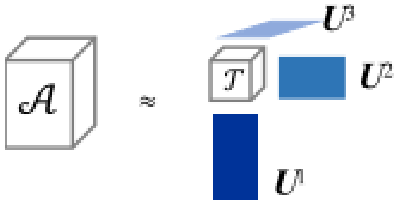

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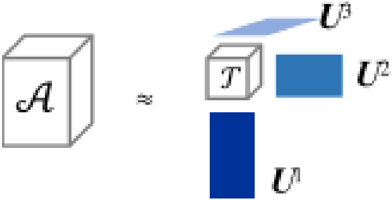

Not generally unique, solved the same as CP decomposition.

Other examples of tensorial PCA methods include:

- 2DPCA
- Generalized low-rank approximation of matrices
- Non-negative MPCA
- Bayesian Tensor Analysis
- Incremental Tensor Analysis
- Dynamic Tensor Analysis
- Window-based Tensor Analysis
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Effectively all generalisations of PCA based on differing objective functions, constraints, and projection methods.

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- Tensorial extensions to ML techniques:
  - Support tensor machine
  - CNNs
  - RNNs
  - Tensor net

Applications

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CP decomposition used to convert tensors into interpretable components $\rightarrow$ factor-matrices. Tucker decomposition used for tensor-compression.

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> *While some chemical engineers have recently been learning about tensorial data analytics, the inspection of the literature indicates that the vast majority have not, as suboptimal methods continue to dominate with no acknowledgement or reference to tensorial methods. Given the sparsity of published applications, there remains little known about which methods to apply to which chemical and biological manufacturing processes, and more detailed application studies need to be clearly documented in the open literature before tensorial data analytics becomes widely accepted and consistently applied in the community.*

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- Data pre-processing procedure for tensorial manufacturing data is key.
- New algorithms are needed to extend flexibility and accuracy of tensor models.
  - Efficient iterative algorithms
  - Optimal initialization
  - Automatic hyperparameter estimation (e.g. components)
  - Sparsity / NN constraints

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- Advanced generalization of process data analytics to tensorial analysis.
  - Non-linear, dynamic and time varying processes.
  - Need to efficiently assess tensorial data properties to inform valid modelling approximations
  - Probabilistic tensorial modelling to incorporate process uncertainties.
  - Should be integrated with process knowledge such as first principles and process structure.

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Image Example

Starting with a third order tensor... an image.
Three orders are width, height and colour(RGB)). With three components.

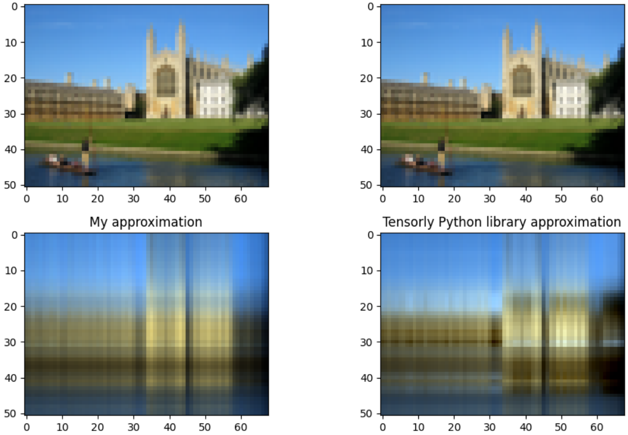


Image Example

With ten components...

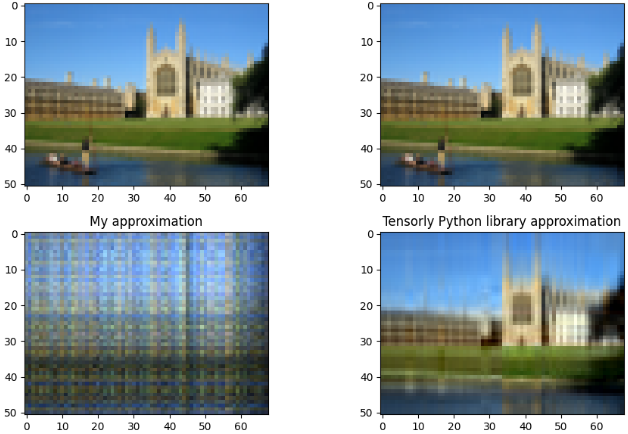
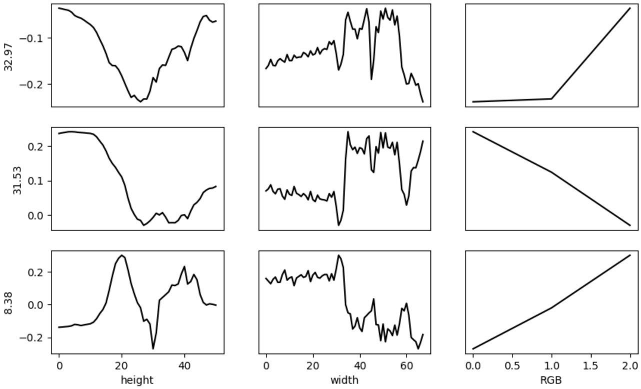


Image Example

Plotting the components of each factor...



Industrial Example