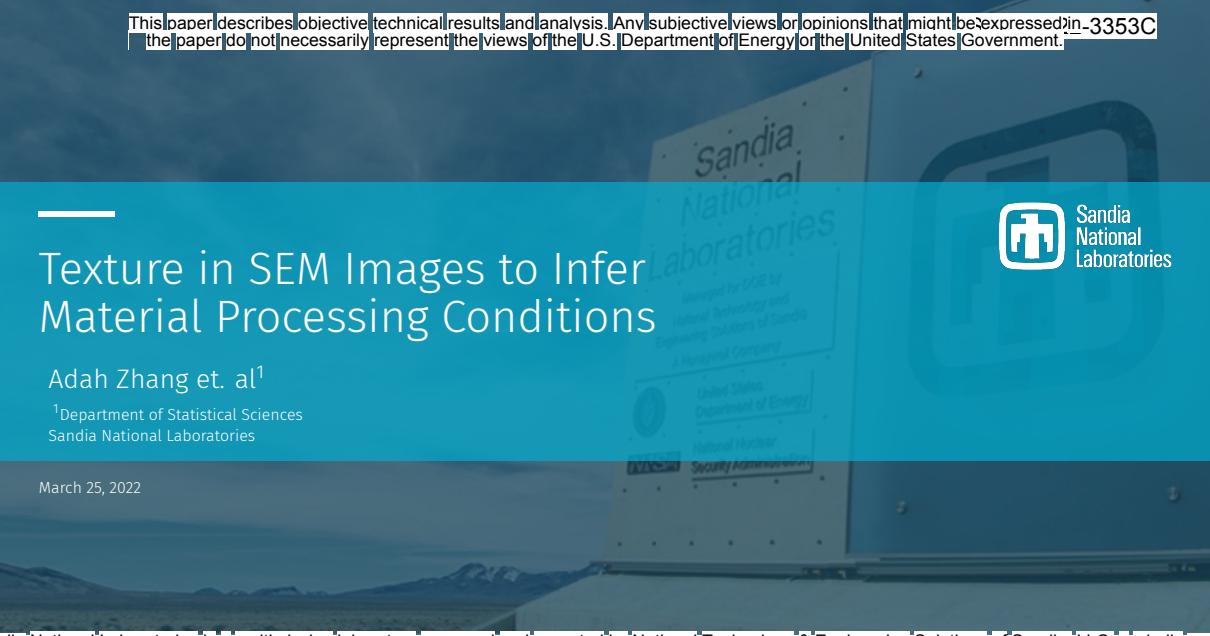

Texture in SEM Images to Infer Material Processing Conditions

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Problem Description

Nuclear Forensics

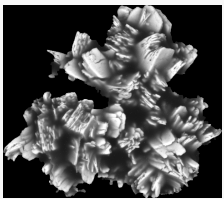
Goal: Identify and attribute a set of processing conditions to interdicted special nuclear materials

- Knowledge about processing conditions is helpful in determining where the material originated
- Identifying processing conditions can be considered an **Inverse Prediction** (IP) problem
  - In classical regression the covariates/predictors are known, and a statistical model is constructed to estimate their relationship with the response
  - In IP problems the goal is to estimate the covariates (processing conditions) using the observed responses
  - Addressed using a **Functional Data Analysis (FDA)** approach from a model incorporating information about particle texture from SEM imagery

Data

Dataset consists of SEM images of particles produced at different processing condition levels of a designed experiment

- The images are segmented and pre-processed to remove noise and background
- Particle texture is influenced by the processing conditions under which the material was produced



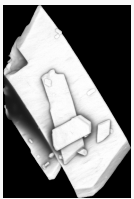
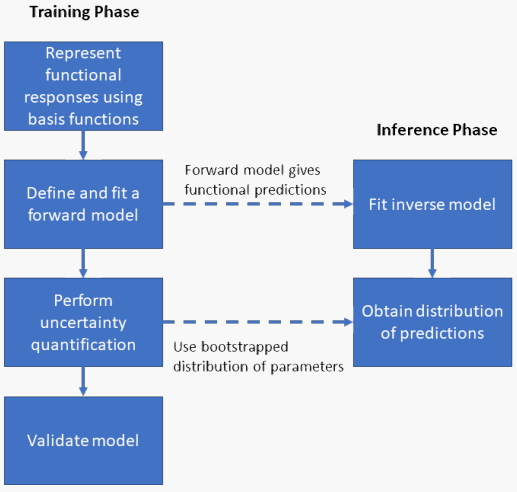


Figure: Contrasting particle textures from different processing conditions

Inference

- The **Functional Inverse Prediction Framework (FIP)** is used to estimate material processing conditions
- FIP model has two stages:
  1. Forward model is fit to training data
  2. Relationships found from forward model are used to estimate unknown covariates from new responses



Model

Forward Model:

$$Y_{ij}(t) = g_j(\mathbf{x}_i; \boldsymbol{\theta}_j(t)) + \epsilon_{ij}(t);\ i = 1, \ldots, n;\ j = 1, \ldots, q,$$

- $g_j(\cdot)$ can be taken to be $\mathbf{x}_i^{'}\boldsymbol{\beta}_j(t)$ for functional linear regression, or other forms for non-linear responses
- $\mathbf{x}_i$ are processing conditions, and $\epsilon_{ij}(t)$ are i.i.d., mean-zero, second-order stationary stochastic processes

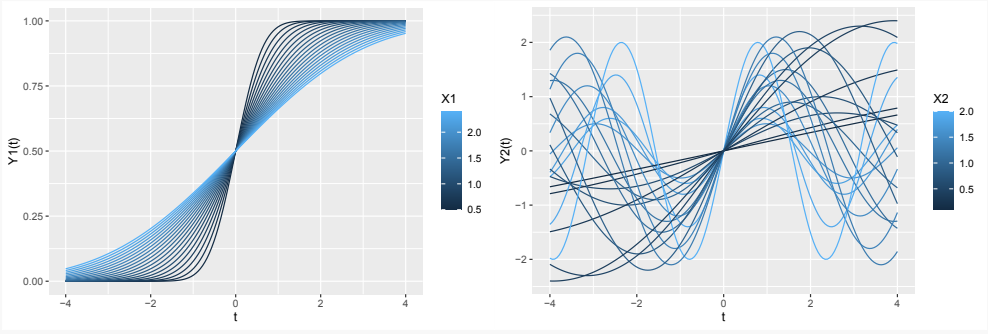
Inverse Model:

$$\hat{\mathbf{x}}^* = \arg\min_{\mathbf{X}^*} \sum_{j=1}^{q} \int L(\hat{y}_j(t), Y_j^*(t))dt,$$

- $\hat{y}_j(t) = g_j(\mathbf{X}^*, \hat{\boldsymbol{\theta}}_j(t))$, $L(\cdot)$ is some loss function, Y_j^* are some new observations/functions

Simulation Study

A simulated functional dataset was produced with two covariates,



$$Y_{i1}(t) = \int_{-\infty}^{t} \frac{1}{\sqrt{2\pi}x_{i1}} e^{-\frac{1}{2x_{i1}^2}u^2} du$$

$$Y_{i2}(t) = x_{i1}\sin(x_{i2}t)$$

- Functional linear model and MARS forward model fit using basis representation

Simulation Study

The Simulation study results indicate the FIP framework is able to recover $\mathbf{x}_1$ and $\mathbf{x}_2$

Table: RMSE for IP of simulation study

	$\mathbf{x}_1$	$\mathbf{x}_2$
Linear	0.06 (0.04)	0.57 (0.26)
MARS	0.02 (0.04)	0.51 (0.26)

Particle Texture to Infer Processing Conditions

The FIP framework was applied to SEM images of particles to infer processing conditions

- Local standard deviation filters were first applied as a pre-processing step to normalize the images and capture features of particle texture not reflected in the raw intensities of the SEM image

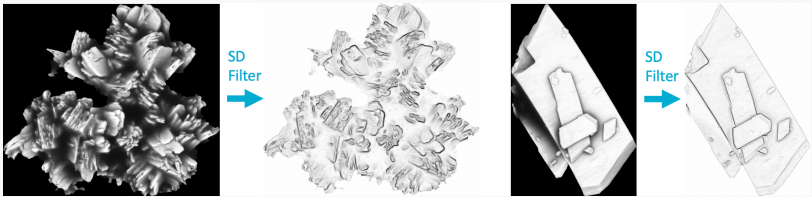
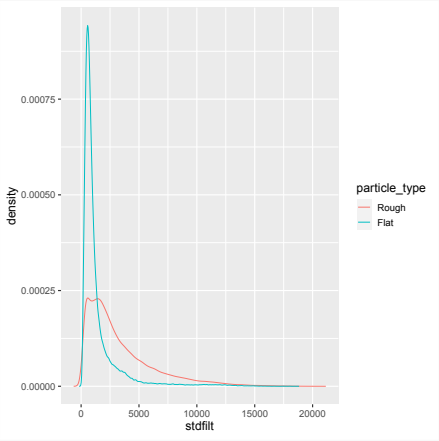
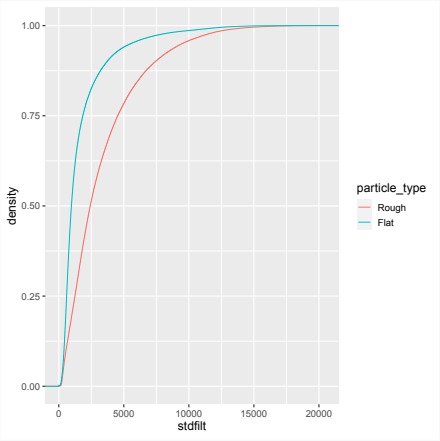


Figure: Particle texture after applying local SD filtering. Darker pixels=Higher SD

Particle Texture to Infer Processing Conditions

CDFs of localized SD values were used as functional responses in the FIP framework





Results: Particle Texture to Infer Processing Conditions

Casting texture information into a functional space is informative for IP of material processing conditions

Table: RMSE of inverse predictions of standardized covariates. Standard errors in parentheses.

Model	Condition 1	Condition 2	Condition 3
Linear	1.18 (0.07)	1.45 (0.10)	1.17 (0.08)
MARS	1.24 (0.39)	1.19 (0.11)	1.25 (0.30)

- Predictions made on a held-out cross validation set
- Uncertainty estimates produced using a bootstrap approach

Conclusion

- FDA approach using texture from SEM images to infer material processing conditions is promising
- Results from FDA modeling of texture are more interpretable than some other black-box models used for image analysis, which is appealing to stakeholders and decision makers
- Combination of texture approach with other feature information (e.g. shape) and more flexible modeling which allows borrowing information across particles may improve inference
- More details on the FIP approach are available in the paper:
  - Ries, D., Zhang, A., Tucker, J. D., Shuler, K., and Ausdemore, M. (February 3, 2022). "A framework for inverse prediction using functional response data." ASME. J. Comput. Inf. Sci. Eng. doi: https://doi.org/10.1115/1.4053752

Thank you for listening!