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# Inverse prediction using functional data in a Bayesian framework

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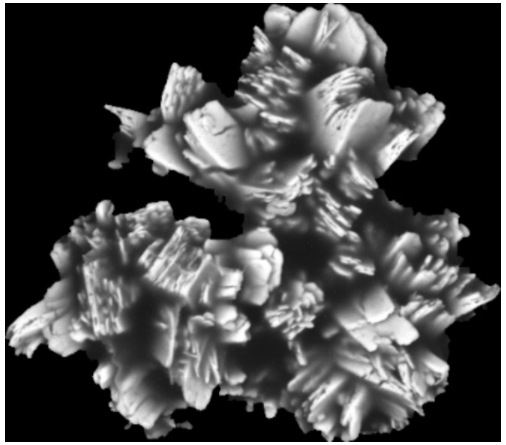
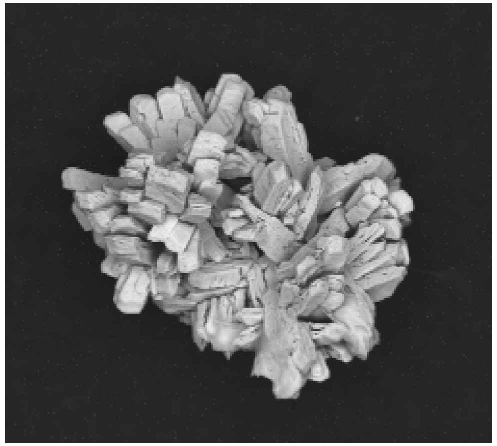
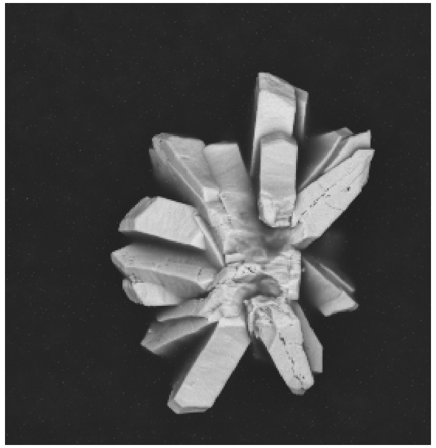
# Modeling Objectives

## Can we predict the processing conditions for this material?





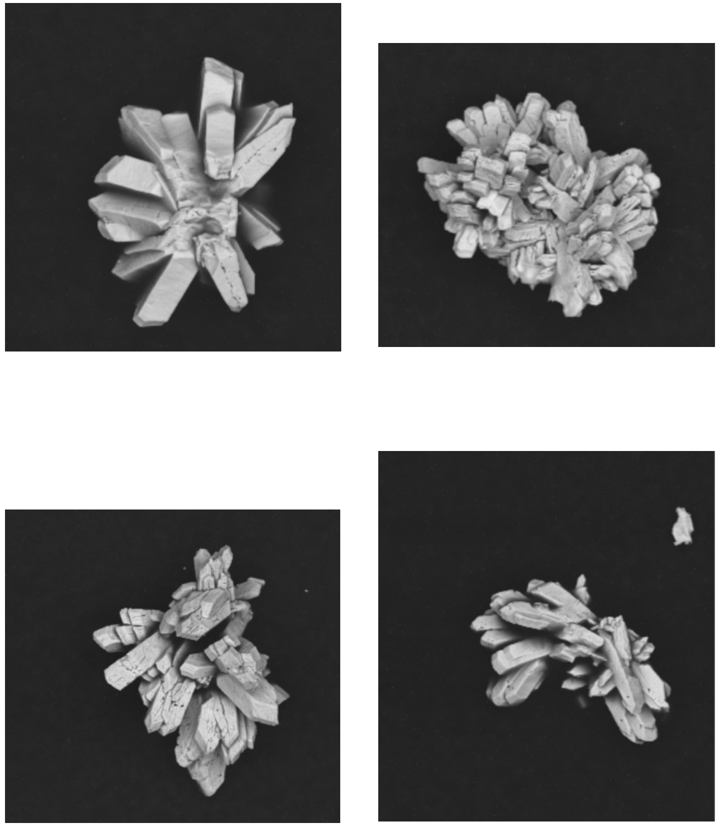


Scanning Electron Microscope (SEM) images of Pu particles

# Modeling Objectives

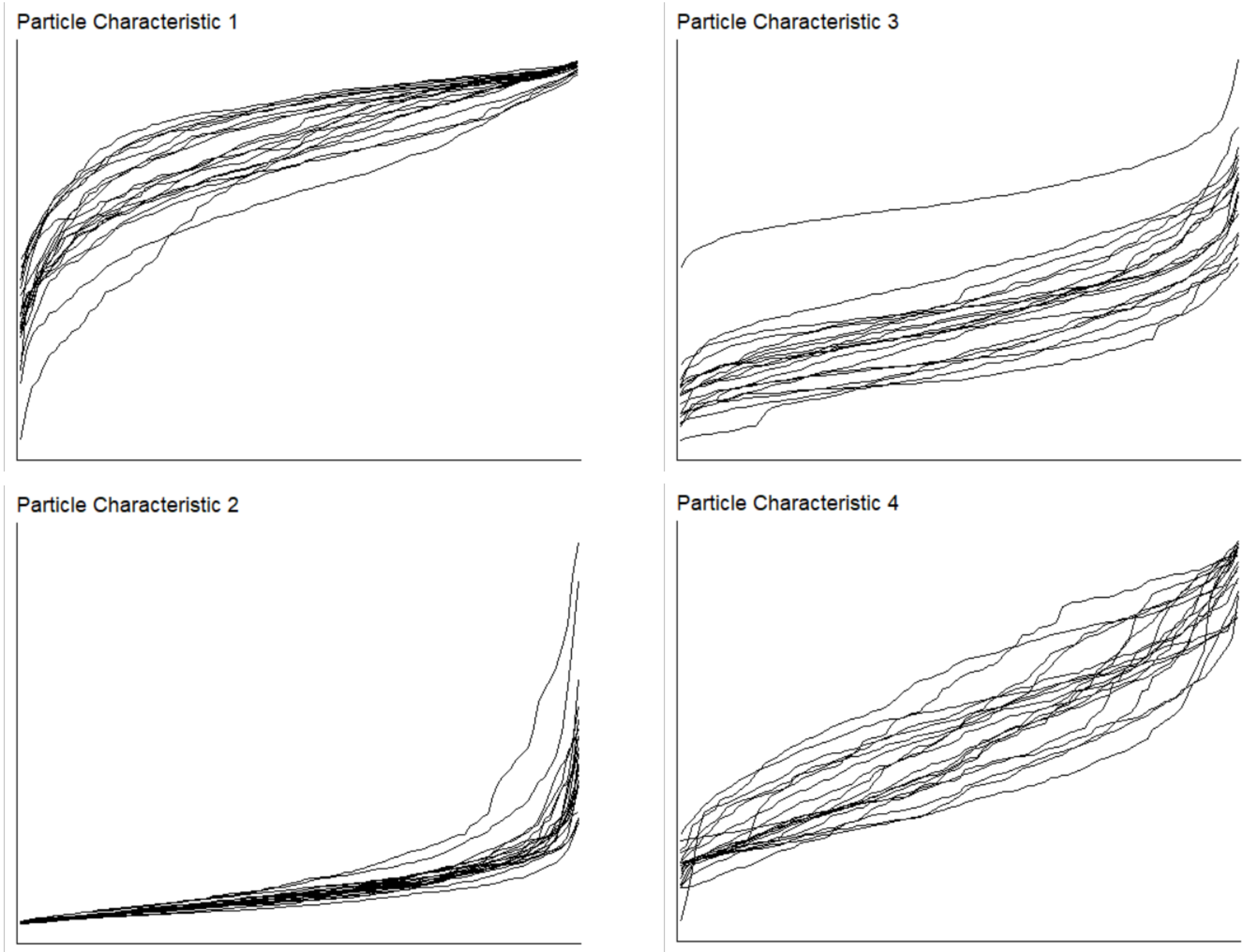
- 4 particle characteristics (e.g., color, texture, size)
- 3 process conditions (e.g., temperature, chemical characteristic, processing time)
- Given the measured particle characteristics, can we predict the exact conditions used to produce the material?
- Project framework:
  - Process Pu under known conditions
  - Measure resulting particle characteristics
  - Fit forward model
  - Inverse-predict test values, quantify uncertainty, and assess predictive accuracy
- Model framework combines:
  - Functional data analysis (FDA)
  - Inverse prediction
  - Seemingly unrelated regression (SUR)
  - Bayesian modeling

# Functional Data



Avg. 640 measurements of each particle characteristic per experimental run

## Empirical CDFs of four particle characteristics



# Functional Inverse Prediction (FIP) framework

1. Represent functional responses using basis functions

fPCA on empirical CDF

2. Fit forward model

Process Condition = *f*(Particle Characteristics) + ε
Determine Particle Characteristics to use in Step 3
Stepwise regression & LASSO

3. Fit inverse model

a) Particle Characteristics = *f*(Process Conditions) + ε
Seemingly Unrelated Regression
b) Predict Processing Conditions
P(Processing Conditions | Particle Characteristics)

4. Validate model

Leave-one-out cross-validation

# Simulated Functional Data

$t \in [-4, 4], n = 150$

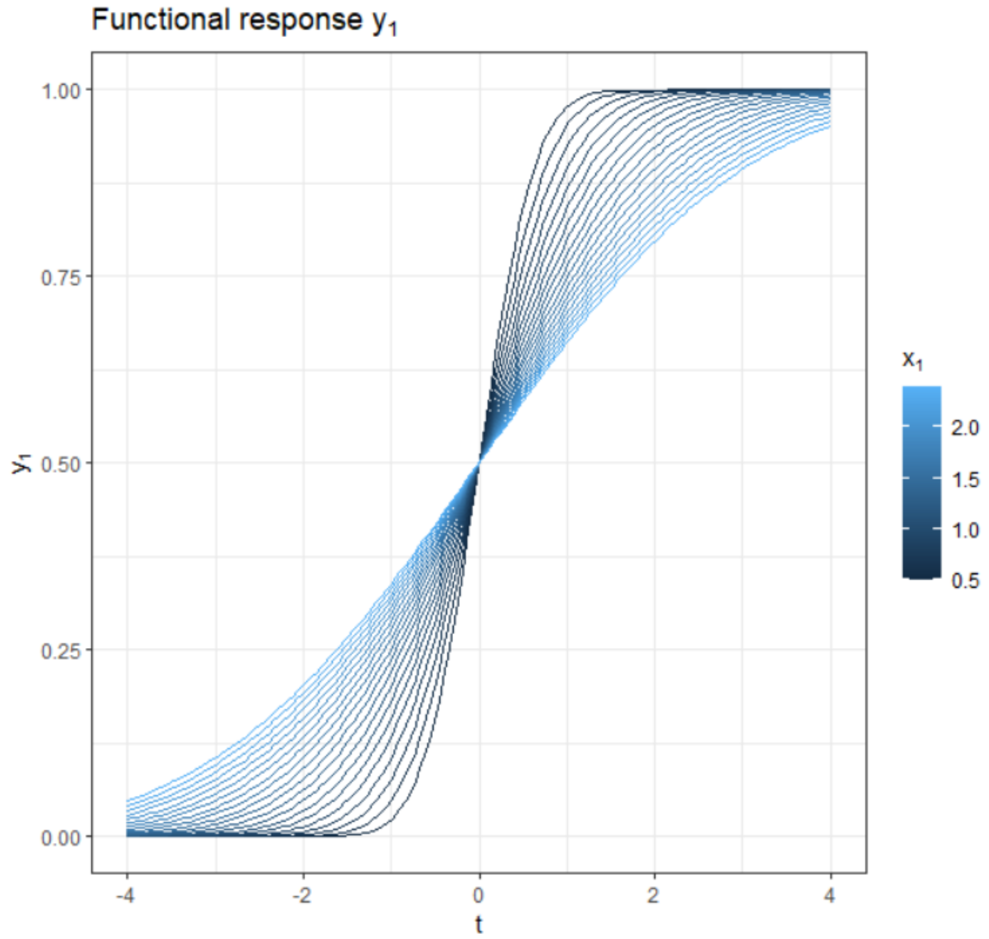
$x_1 \in [0.5, 2.4], n = 20$

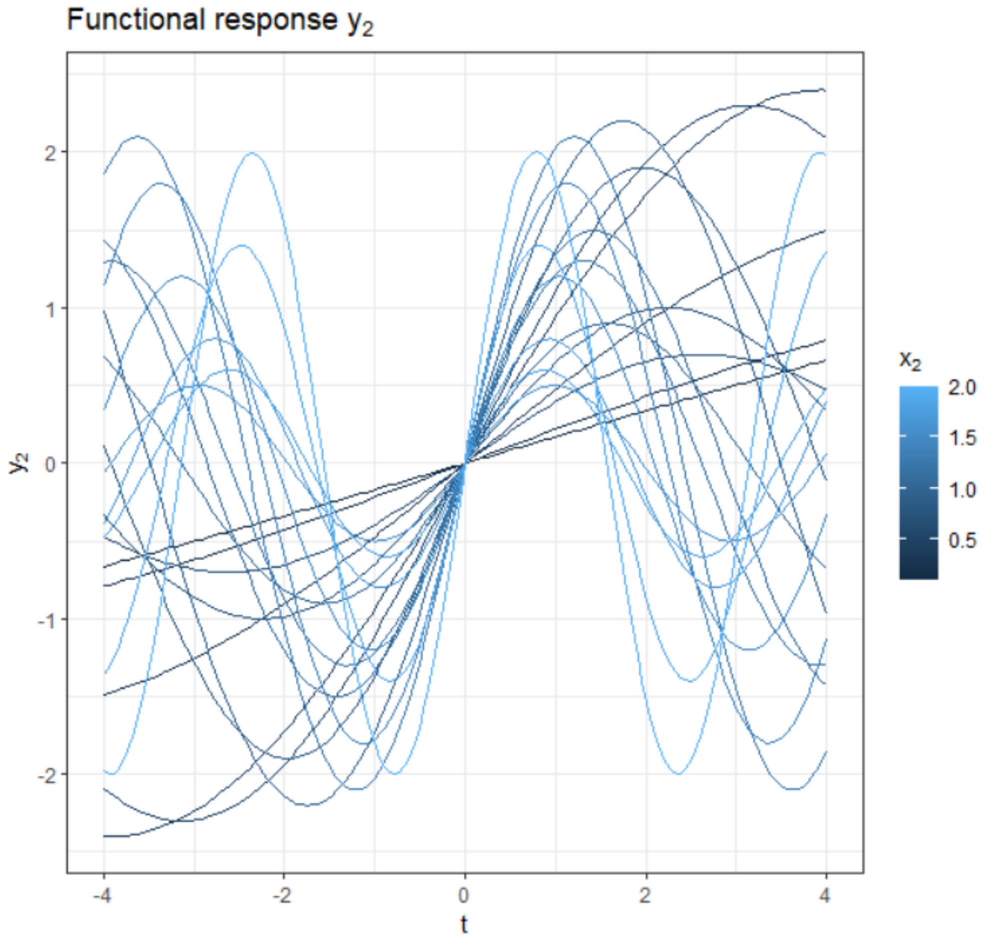
$x_2 \in [0.1, 2], n = 20$

$y_1 = \Phi_t(0, x_1)$

$y_2 = x_1 \sin(x_2 t)$

Use first two principal components (PCs) as response variables (4 total)



# Functional Inverse Prediction (FIP)

<u>Model:</u>

$$y_{q,i}^{k} = \beta_{0qk} + \beta_{1qk}x_{1,i} + \beta_{2qk}x_{2,i} + \epsilon_{q,i}^{k}$$

Principal Component $k \in \{1, 2\}$ from response variable $y_q, q \in \{1, 2\}$ and observation $i \in \{1, \ldots, 20\}$

<u>Bayesian Implementation:</u>

For inverse-predicting $x_{1,1}$ and $x_{2,1}$

$$\begin{bmatrix} \mu_{q,1}^{k} \\ \mu_{q,2}^{k} \\ \vdots \\ \mu_{q,n}^{k} \end{bmatrix} = \beta_{0qk} + \beta_{1qk}\begin{bmatrix} NA \\ x_{1,2} \\ \vdots \\ x_{1,n} \end{bmatrix} + \beta_{2qk}\begin{bmatrix} NA \\ x_{2,2} \\ \vdots \\ x_{2,n} \end{bmatrix}$$

$$y_{q,i}^{k} \sim N\left(\mu_{q,i}^{k}, \tau_{qk}\right)$$

Standard priors on $\boldsymbol{\beta}$ and $\boldsymbol{\tau}$

Data: $\boldsymbol{X}, \boldsymbol{Y}$ matrices

Estimated: $\boldsymbol{\mu}, \boldsymbol{\beta}, \boldsymbol{\tau}$ matrices

# Simulated Data Results: FIP

$$y^k_{q,i} = g(\boldsymbol{X_q \beta_q}) + \epsilon^k_{q,i}$$

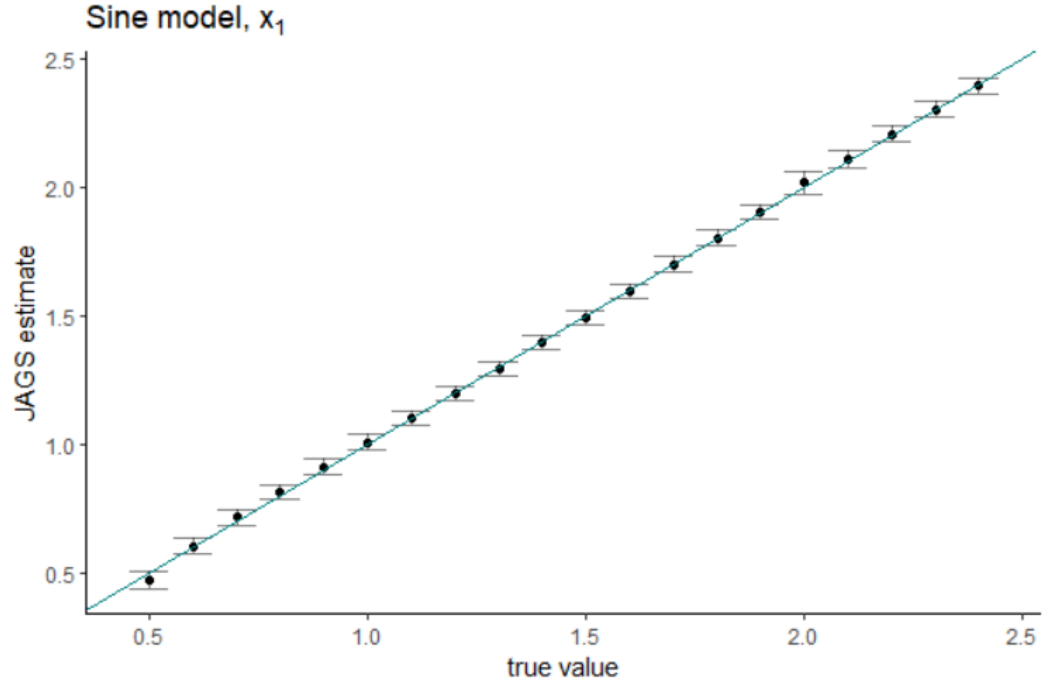
Linear model: $\beta_0 + \beta_1 x_1 + \beta_2 x_2$

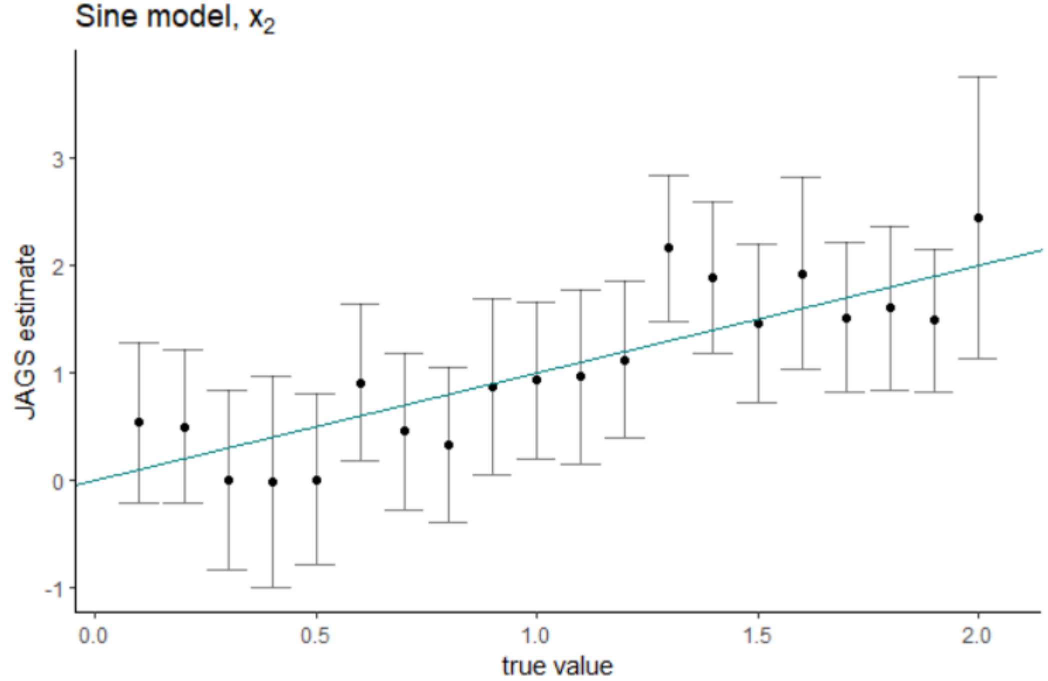
Interaction model: $\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2$

Quadratic model: $\beta_o + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_2^2$

Sine model: $\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 \sin(x_2)$

| Model | RMSE $x_1$ | RMSE $x_2$ |
|---|---|---|
| Linear | 0.044 | 0.479 |
| Interaction | 0.021 | 1.559 |
| Quadratic | 0.011 | 0.398 |
| Sine | 0.011 | 0.392 |



# Seemingly Unrelated Regression (SUR)

- Generalization of simple linear regression
- Looks like multiple regression
  - Response is $n \times Q$ matrix $\boldsymbol{Y}$ composed of $\boldsymbol{Q}$ response variables $\boldsymbol{y}_q, q = 1, \ldots Q$
- Each response variable $\boldsymbol{y}_q$ has its own regression equation
  - Possibly (usually) different predictors, different regression functions (e.g. linear, quadratic) associated with each regression equation
- Error terms across regression equations are allowed to be correlated
  - For response vectors $\boldsymbol{y}_q$and $\boldsymbol{y}_{\boldsymbol{r}}$
    - $cor(y_{qi}, y_{qj}) = 0$ Observations within a response are independent
    - $cor(y_{qi}, y_{ri}) \neq 0$ Observations across responses can be correlated

# Seemingly Unrelated Regression

$$\boldsymbol{y}_q = \boldsymbol{X}_q \boldsymbol{\beta}_q + \boldsymbol{\epsilon}_q$$

$\boldsymbol{y}_q$ is $n \times 1$

$\boldsymbol{X}_q$ is $n \times p_q$

$\boldsymbol{\beta}_q$ is $p_q \times 1$

$\boldsymbol{\epsilon}_q$ is $n \times 1$

$p_q$ is the number of predictors in regression equation $q$

## Stacked

$$\underset{nQ\times 1}{\begin{bmatrix} \boldsymbol{y}_1 \\ \boldsymbol{y}_2 \\ \vdots \\ \boldsymbol{y}_Q \end{bmatrix}} = \underset{nQ\times \sum_Q p_q}{\begin{bmatrix} \boldsymbol{X}_1 & \cdots & 0 \\ 0 & \ddots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & \boldsymbol{X}_Q \end{bmatrix}} \underset{\sum_Q p_q \times 1}{\begin{bmatrix} \boldsymbol{\beta}_1 \\ \boldsymbol{\beta}_2 \\ \vdots \\ \boldsymbol{\beta}_Q \end{bmatrix}} + \underset{nQ\times 1}{\begin{bmatrix} \boldsymbol{\epsilon}_1 \\ \boldsymbol{\epsilon}_2 \\ \vdots \\ \boldsymbol{\epsilon}_Q \end{bmatrix}}$$

## Covariance structure

$cov(\epsilon_{qi}, \epsilon_{qj}) = 0 \; for \; i \neq j$ observation

$cov(\epsilon_{qi}, \epsilon_{ri}) \neq 0 \; for \; q \neq r$ regression

$$\underset{Q\times Q}{\Sigma} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \dots & \sigma_{1Q} \\ \sigma_{21} & \sigma_{22} & & \sigma_{2Q} \\ \vdots & & \ddots & \vdots \\ \sigma_{Q1} & \sigma_{Q2} & \cdots & \sigma_{QQ} \end{bmatrix}, \sigma_{qr} = cov(\epsilon_{qi}, \epsilon_{ri}) \, \forall i$$

$$\Omega = \Sigma \otimes I_n$$

$nQ \times nQ$ block matrix whose blocks are diagonal matrices

# Simulated Data with Correlated Errors

## Covariance structure

$cov(\epsilon_{qi}, \epsilon_{qj}) = 0 \ for \ i \neq j$ observation

$cov(\epsilon_{qi}, \epsilon_{qj}) = 1 \ for \ i = j$ observation

$cov(\epsilon_{qi}, \epsilon_{ri}) = 0.9 \ for \ q \neq r$ regression

$$\Sigma = \begin{bmatrix} \sigma_{11} = 1 & \sigma_{12} = 0.9 \\ \sigma_{12} = 0.9 & \sigma_{22} = 1 \end{bmatrix}$$

$$\Omega = \Sigma \otimes I_{20}$$

## Uncorrelated simulated data

$t \in [-4, 4], n = 150$

$x_1 \in [0.5, 2.4], n = 20$

$x_2 \in [0.1, 2], n = 20$

$y_1 = \Phi_t(0, x_1)$

$y_2 = x_1 \sin(x_2 t)$

## Correlated simulated data

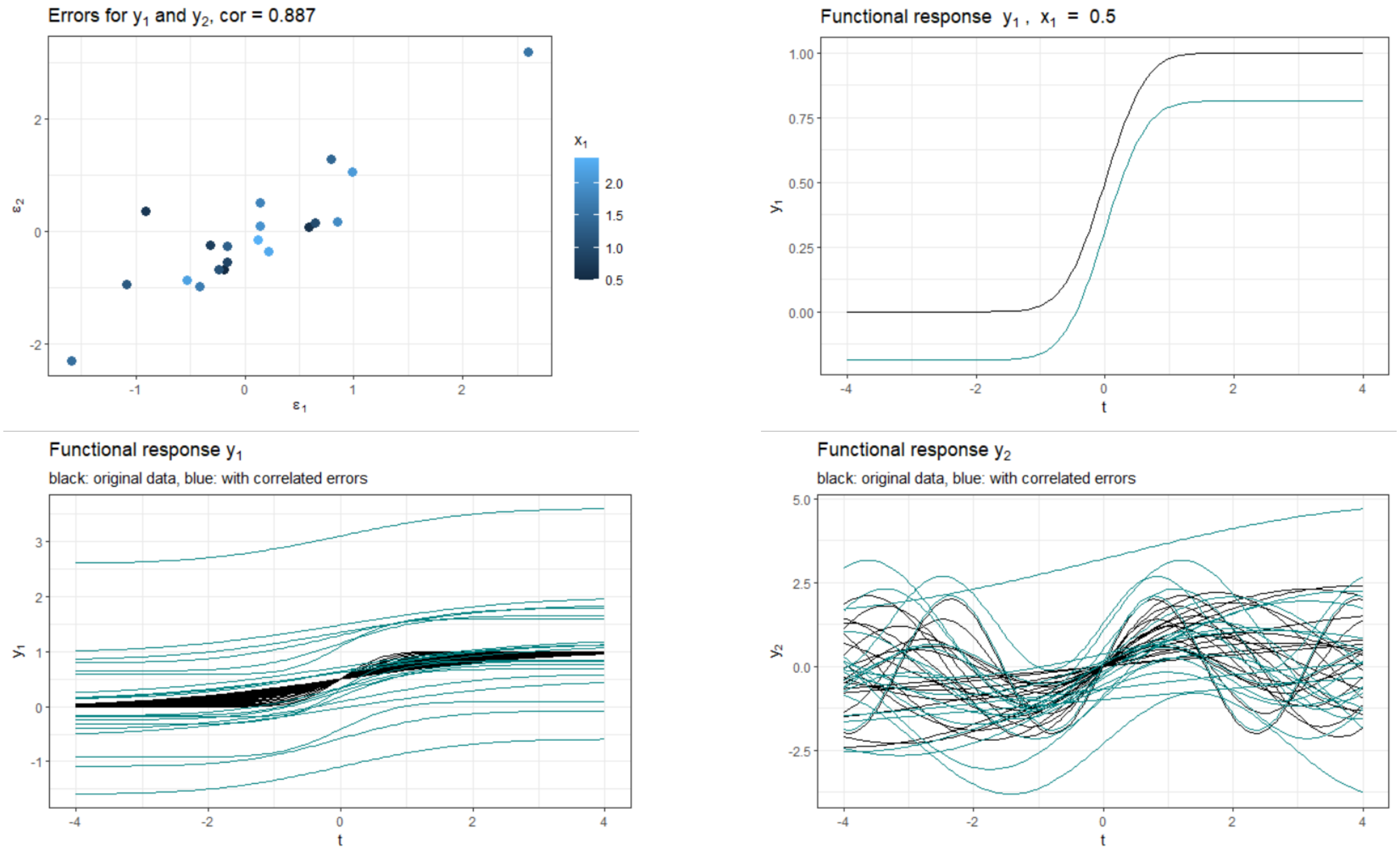
$\epsilon_q \sim \mathrm{MVN}(\mathbf{0}, \Omega)$

$\boldsymbol{y}_1^* = \boldsymbol{y}_1 + \boldsymbol{\epsilon}_1$

$\boldsymbol{y}_2^* = \boldsymbol{y}_2 + \boldsymbol{\epsilon}_2$

Use first two PCs as response variables (4 total)

# Simulated Data with Correlated Errors



# Correlated Simulated Data Results: FIP with SUR

Correlated errors

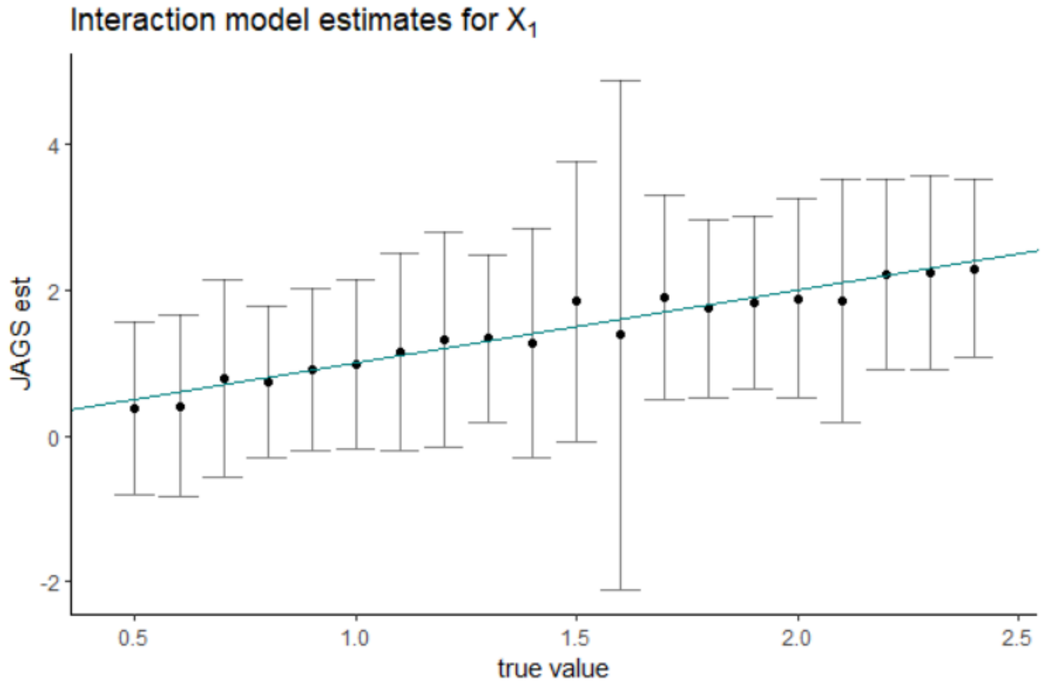
$$y^k_{q,i} = g(\boldsymbol{X_q \beta_q}) + \epsilon^k_{q,i}$$

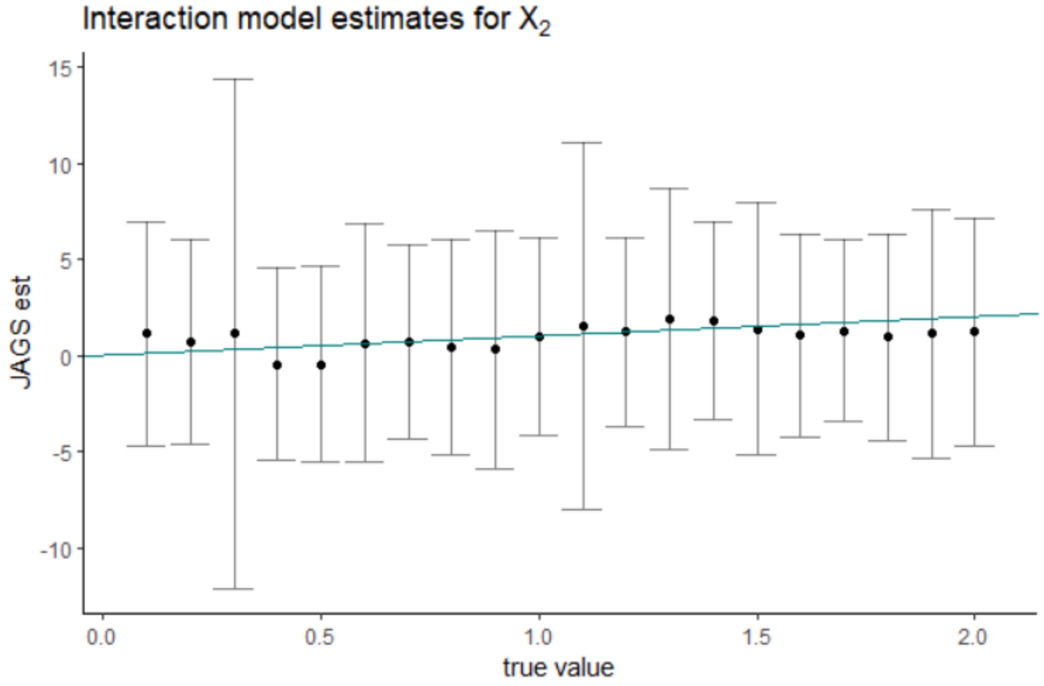
Interaction model: $\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2$

Quadratic model: $\beta_o + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1^2 + \beta_4 x_2^2$

Sine model: $\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 \sin(x_2)$

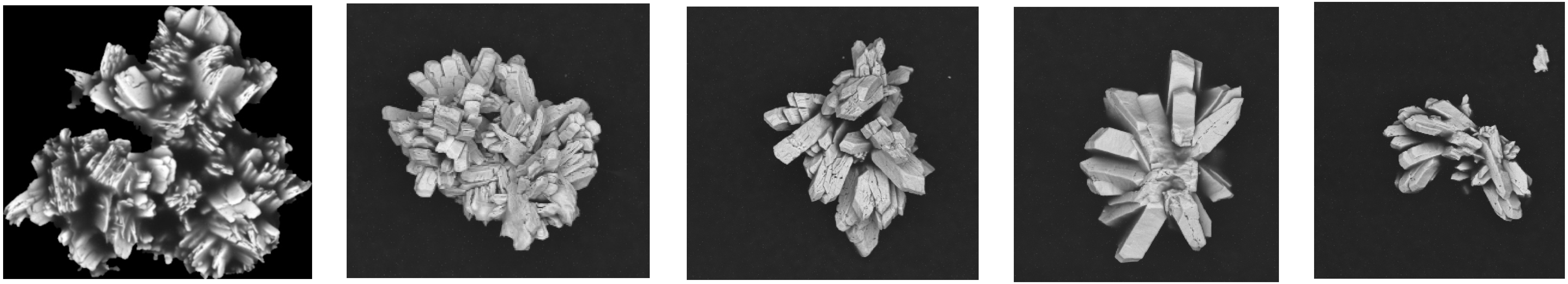
| Model | RMSE $x_1$ | RMSE $x_2$ |
|---|---|---|
| Interaction | 0.141 | 0.602 |
| Quadratic | 0.171 | 0.782 |
| Sine | 0.171 | 0.893 |



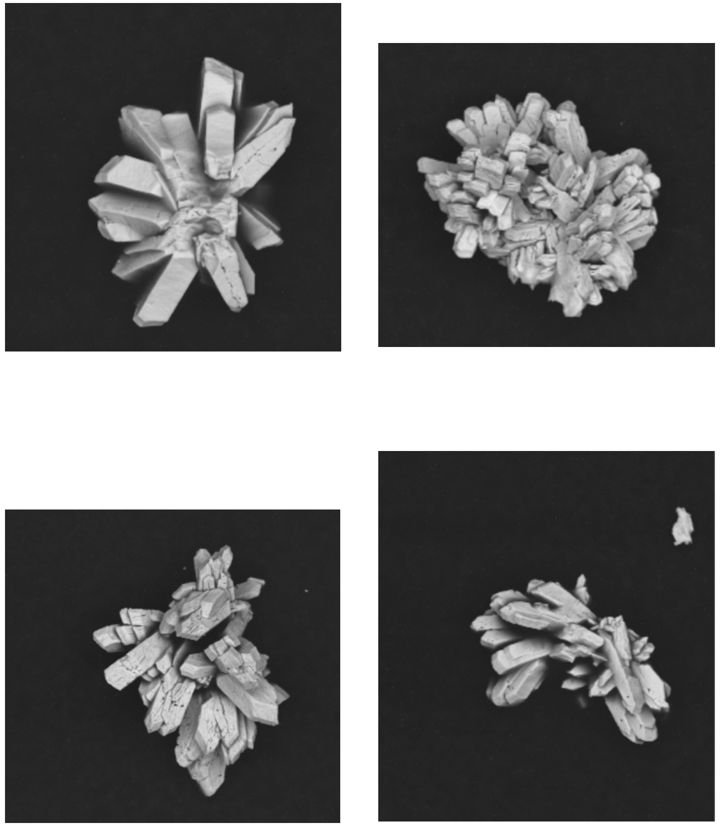
# Can we predict the processing conditions for this material?

- 4 particle characteristics (e.g., color, texture, size)
- 3 process conditions (e.g., temperature, chemical characteristic, processing time)



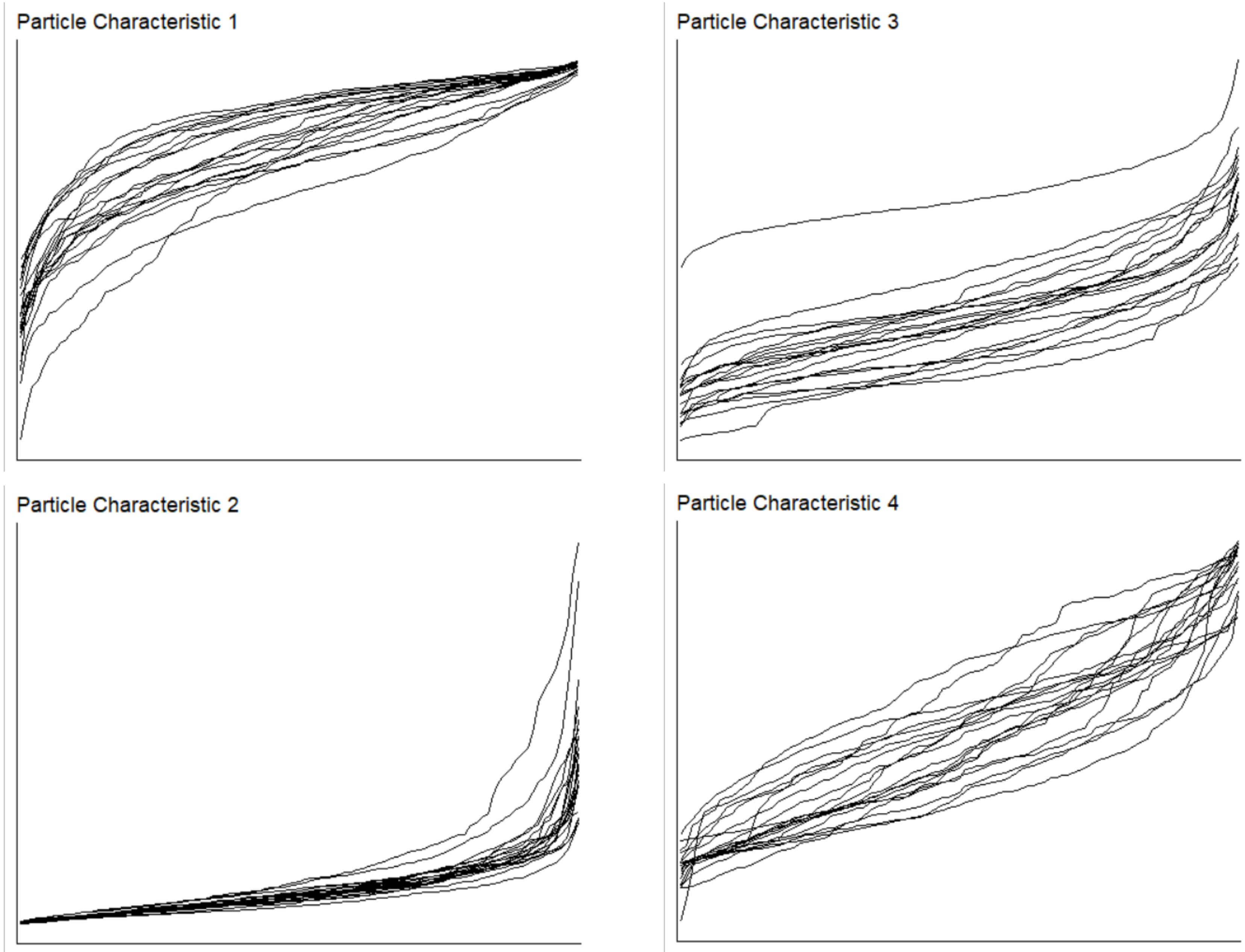
SEM images of Pu particles

# Functional Data



Avg. 640 measurements of each particle characteristic per experimental run

## Empirical CDFs of four particle characteristics



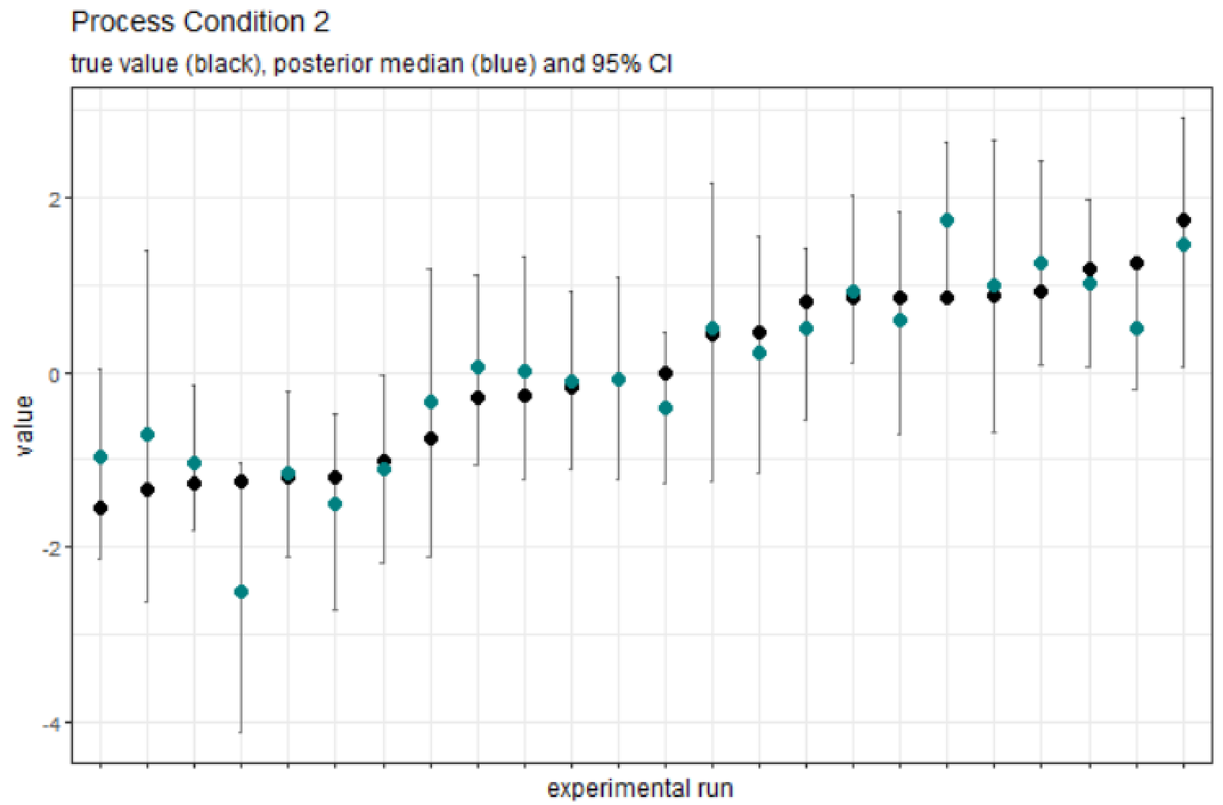
# Implementation

- Forward model: Process Condition = *f*(Particle Characteristics) + ε
  - Identify Particle Characteristics associated with each Process Condition
  - Stepwise regression and LASSO
  - e.g., Particle Characteristics 2 & 3 identified as important for Process Condition 1
- Inverse Model: Particle Characteristics = *f*(Process Conditions) + ε
  - Bayesian implementation of SUR
  - Y matrix: PCs of Particle Characteristics
  - X Matrix: Process Conditions
  - “Masking” matrix
- Four inverse models:
  - Linear
  - Quadratic
  - 2 interaction models

# SUR results

RMSEs for best model. A value of 1 indicates parity with mean-only model.

| Model | Process Cond. 1 | Process Cond. 2 | Process Cond. 3 |
|---|---|---|---|
| Linear | 0.996 | 0.589 | 0.958 |
| Quadratic | 0.974 | 0.525 | 0.883 |
| Interaction (sparse) | 1.014 | 0.592 | 1.097 |
| Interaction (full) | 1.162 | 0.450 | 0.987 |



# Conclusions

- Functional inverse prediction (FIP) framework successfully extended to Seemingly Unrelated Regression (SUR) in a Bayesian context
- MCMC interpolates missing data to perform inverse prediction
- Identification of "important" predictors in forward model (LASSO and stepwise regression) is somewhat subjective. Stepwise regression seemed to do a better job with our data.
- Results on simulated data are promising, although key simplifying assumption is important
  - Further work needed to develop framework for generating correlation matrix $\Omega$ in a functional context
- Results on actual data are more limited, although when it works, it works well.

# Acknowledgements

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# References


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