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A Functional Statistical Modeling Approach to Using Plutonium Particle Features from SEM Images

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Problem Description

Goal of Nuclear Forensics: 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 Inverse Prediction** (FIP) framework from model incorporating information on particle features from SEM imagery.

Data

SEM images of particles were produced at different processing conditions levels specified from an I-optimal statistically designed experiment [1].

- The images were segmented and pre-processed to remove noise and background.
- MAMA morphological software was used to collect scalar features (measures of area, perimeter, major ellipse/minor ellipse, aspect ratio, etc.) for each particle and the response by run was represented by CDFs of the scalar features [2][3].
- Particle features are influenced by the processing conditions under which the material was produced.

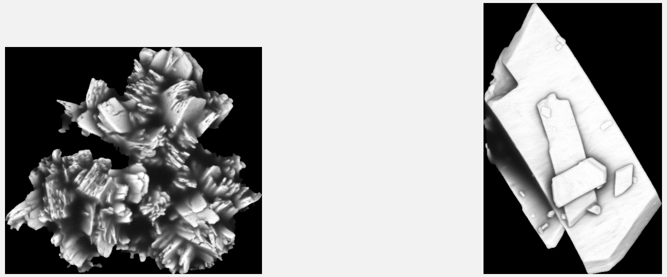


Fig.1: Contrasting particle features from different processing conditions.

Distributions of MAMA Measurements

X-axis: MAMA Characteristic
Y-axis: Cumulative Density Function (CDF)

Blue shading: True value of Condition 1 processing condition across *all* runs
Red line: True distribution of particles from a *single* run

These distributions can be treated as functions and modeled to discriminate between processing conditions.

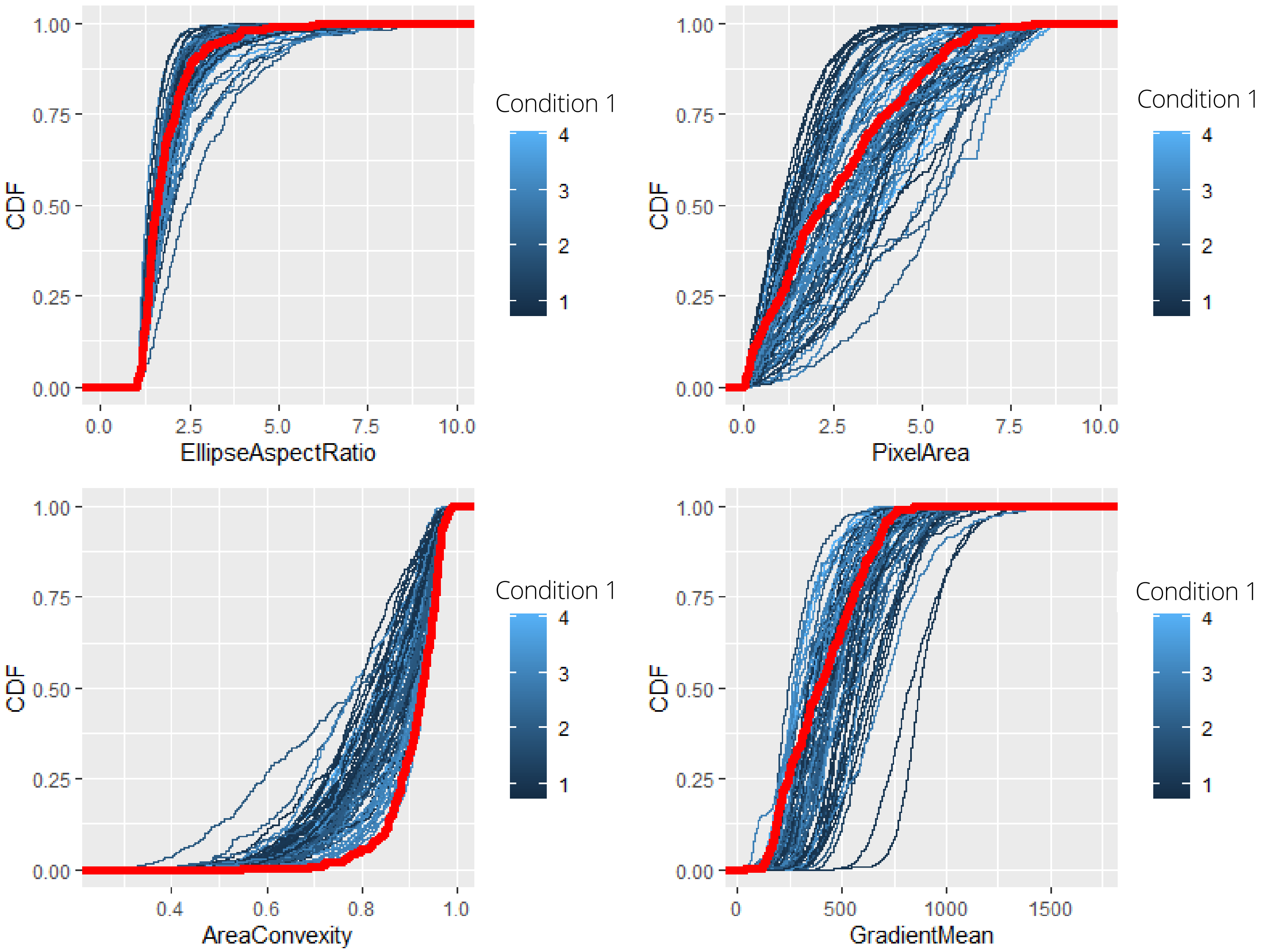


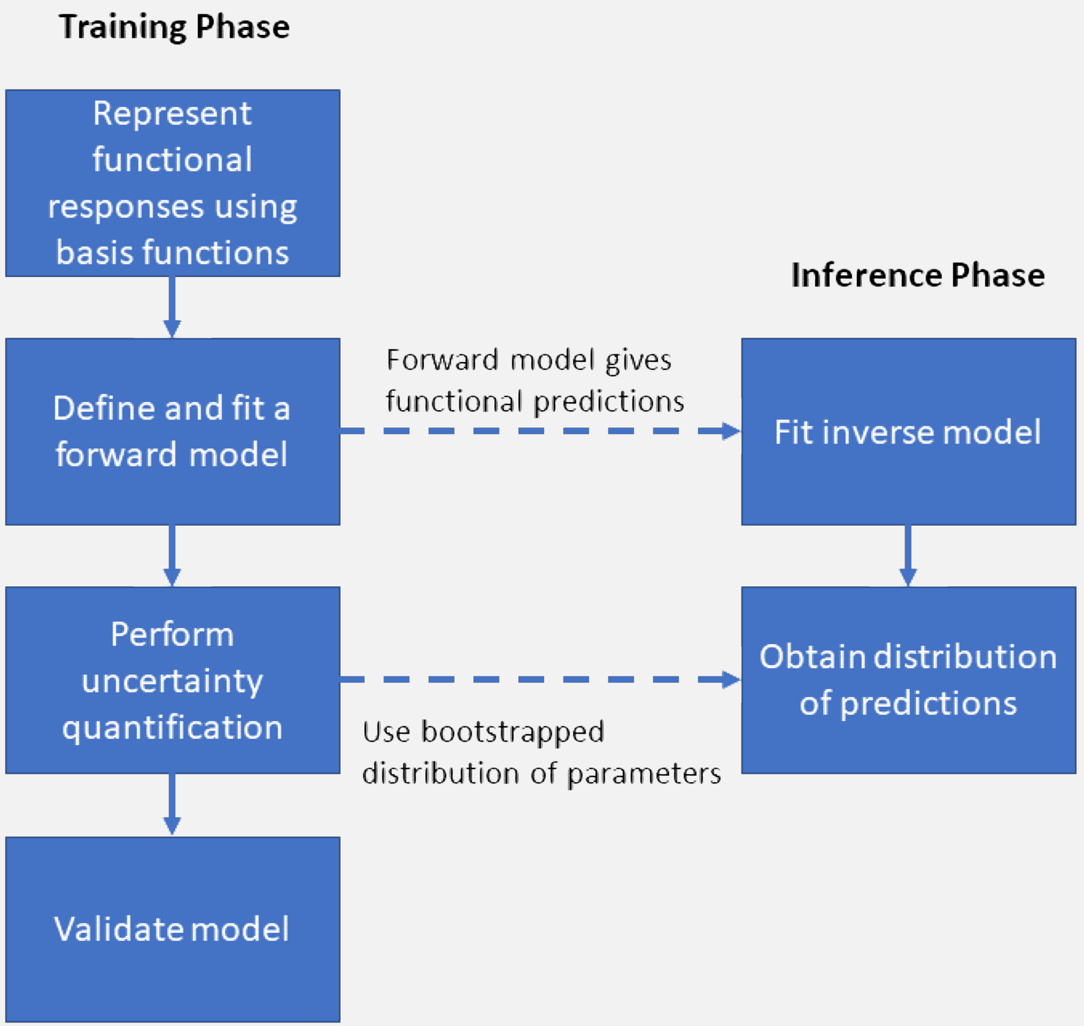
Fig. 2: Demonstration of representing CDFs of MAMA characteristics as functions.

Inference

The Functional Inverse Prediction (FIP) framework [4] is used to estimate material processing conditions, which 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

Fig. 3: Functional Inverse Prediction Framework.



Model

Forward Model:

$$Y_{ij}(t) = g_j\left(x_i; \theta_j(t)\right) + \epsilon_{ij}(t); i = 1, \dots, n; j = 1, \dots, q, \text{ where}$$

- $g_j(\cdot)$ can be taken to be $x_i' \beta_j(t)$ for functional linear regression, or other forms for non-linear responses
- x_i are processing conditions and $\epsilon_{ij}(t)$ are i.i.d., mean-zero, second-order stational stochastic processes

Inverse Model:

$$\hat{x}^* = \underset{X^*}{\operatorname{argmin}} \sum_{j=1}^{q} \int L(\hat{y}_j(t), Y_j^*(t))dt, \text{ where}$$

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

Simulation Study

A simulated functional dataset was produced with two covariates,

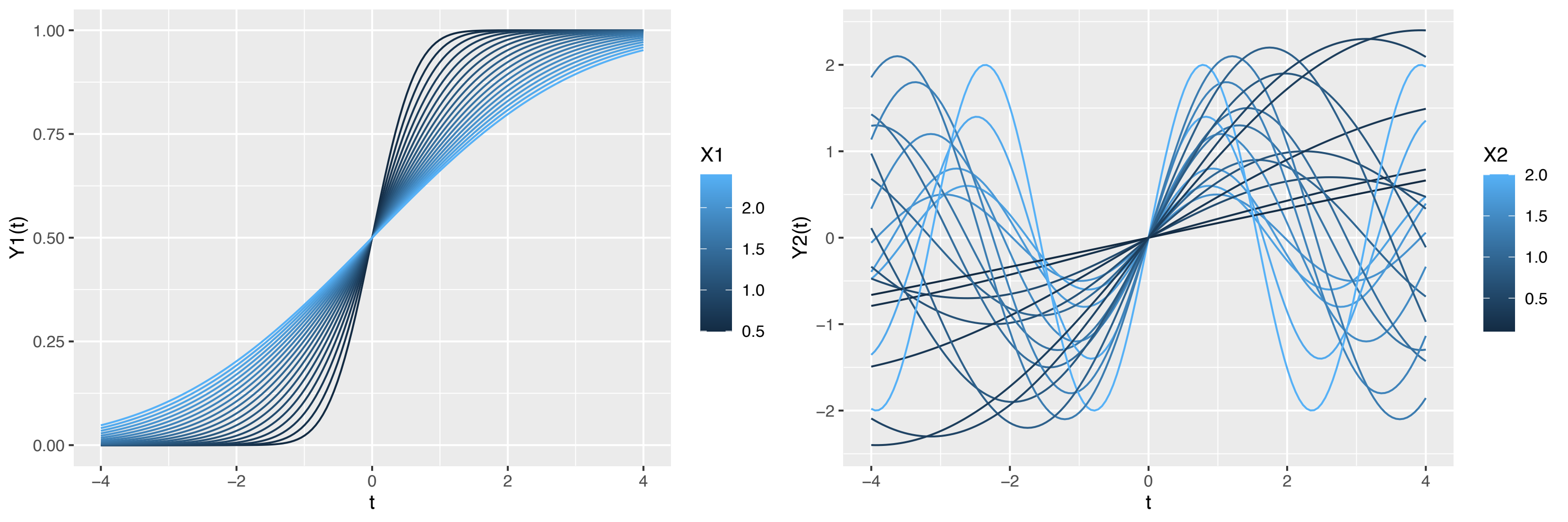


Fig. 4: Functional responses, Y1 and Y2, from simulated dataset.

$$Y_{i1}(t) = \int_{-\infty}^{t} \frac{1}{\sqrt{2\pi x_{i1}}} e^{-\frac{1}{2x_{i1}^2}u^2} du \qquad\qquad Y_{i2}(t) = x_{i1}\sin(x_{i2}t)$$

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

Simulation Study Results

The simulation study results indicate that the FIP framework is able to recover x_1 and x_2

Tab. 1: RMSE for IP of simulation study

	x_1	x_2
Linear	0.06 (0.04)	0.57 (0.26)
MARS	0.02 (0.04)	0.51 (0.26)

RMSE = standard deviation of the residuals

Approaches for FIP

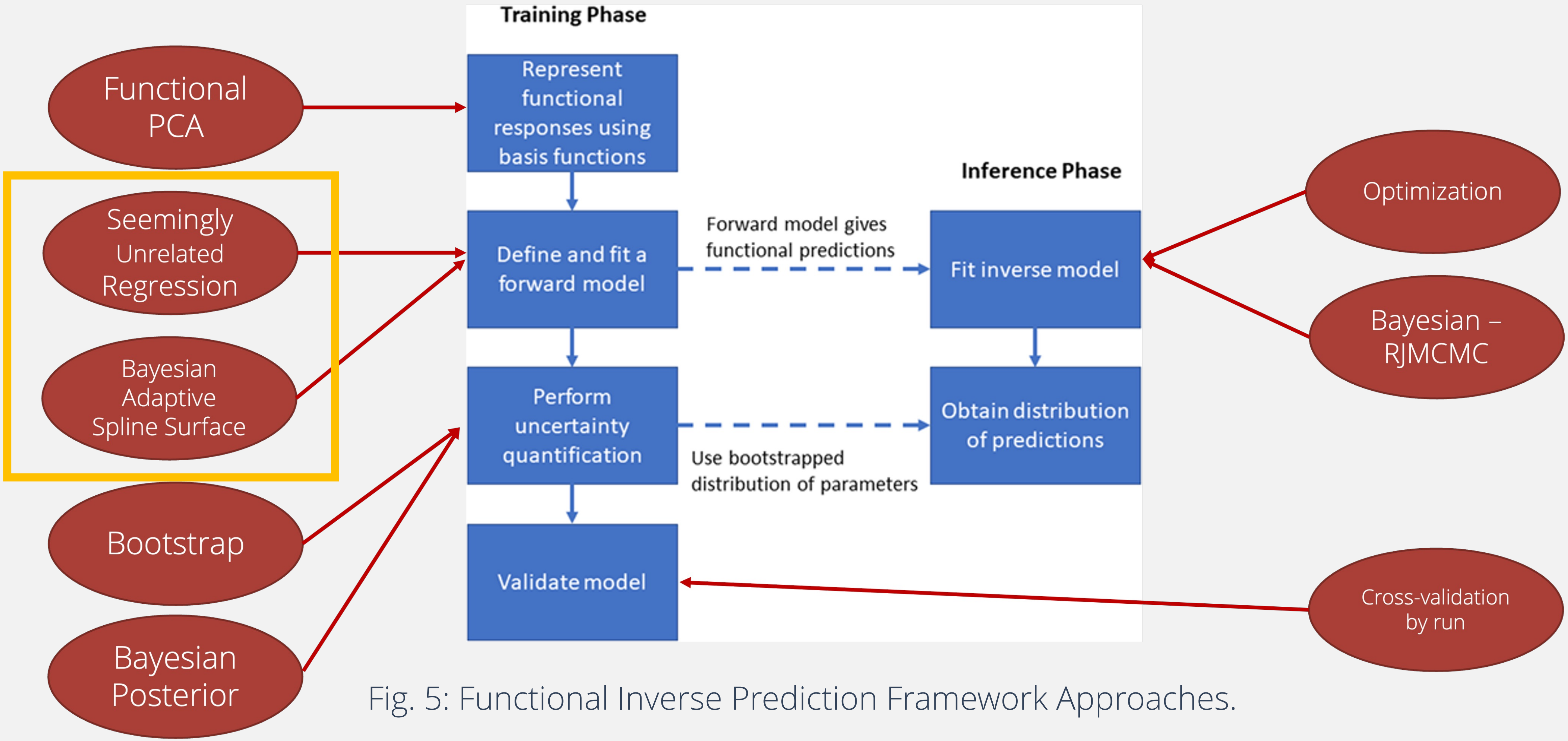


Fig. 5: Functional Inverse Prediction Framework Approaches.

Seemingly Unrelated Regression

- A generalization of a linear regression model that contains only exogenous regressors (only related through the error terms).
- Fit forward and inverse model
- Fit into a Bayesian framework for easy UQ
- Considers particles within a run as a group
- Accounts for correlations between errors in morphological characteristics. I.e. for a particular run with the same set of processing conditions, morphological characteristics, such as particle size, shape, and smoothness are likely related.

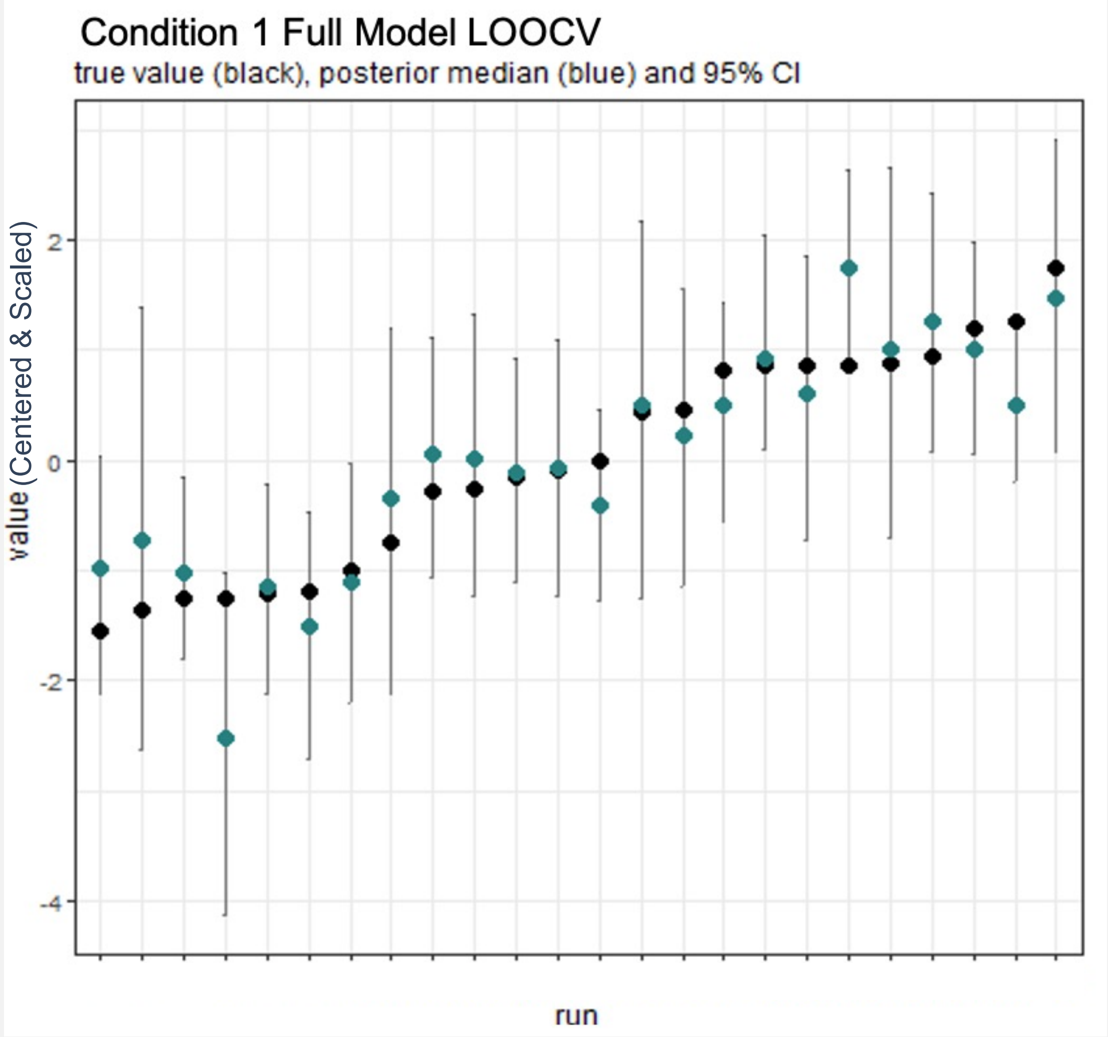
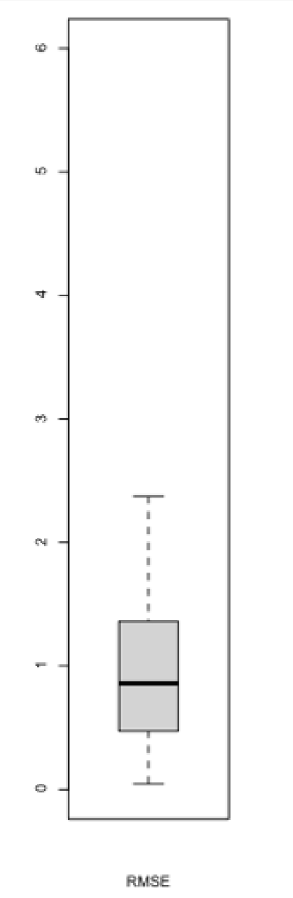


Fig. 6: Model performance assessment using LOOCV on SUR for Condition 1.

Bayesian Adaptive Spline Surface

- A non-linear model for nonparametric regression that incorporates flexibility, scalability, interpretability, and probabilistic accuracy.
- Fit a direct model
- Fits in a Bayesian framework for easy UQ
- Considers particles within a run individually, then combines results post hoc.

Fig. 7: BASS RMSE of Condition 1 for all particles



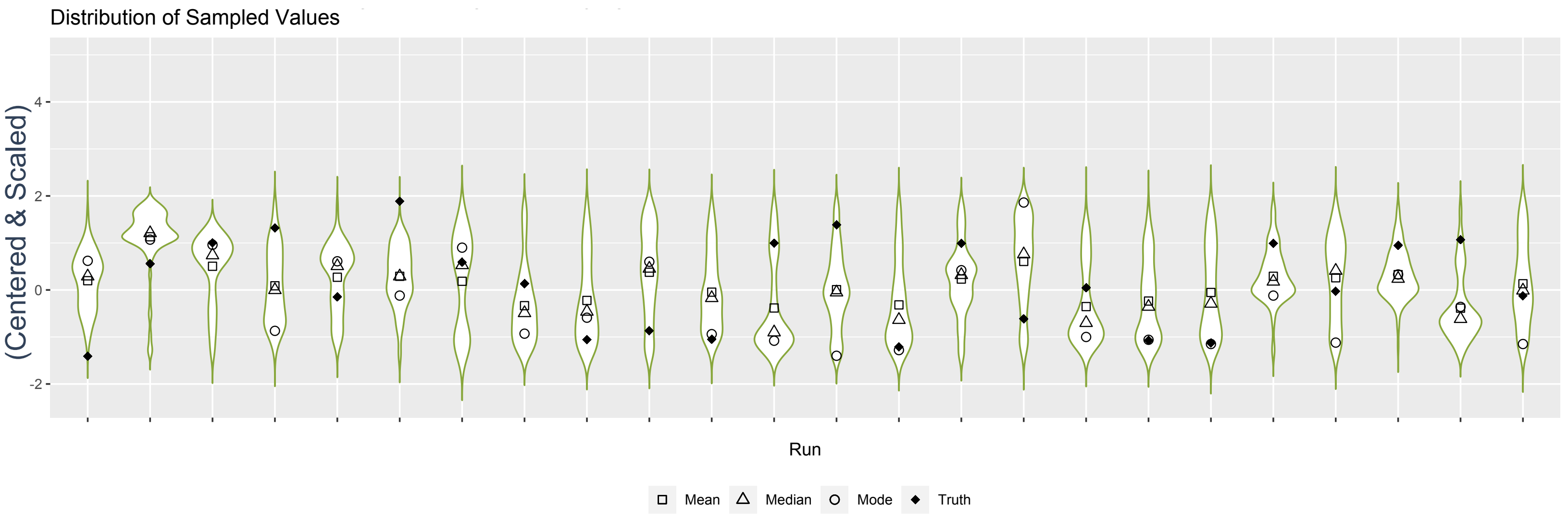


Fig. 8: Model performance assessment using LOOCV on BASS for Condition 1.

Conclusion

- There is a lot of variability in the chemical process that it makes it difficult to parse out the signal from noise in a purely-data driven manner.
- Non-linear relationships exist between processing conditions and particle features.
- Models are constructed so they are interpretable, allowing us to understand which particle features affect which processing conditions.
- Models are only as good as the data– if the major sources of variability are not captured in the data, then it will be difficult to develop generalizable data-driven models.
- Uncertainties on predictions are relatively large for all models considered.

Thank you!

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