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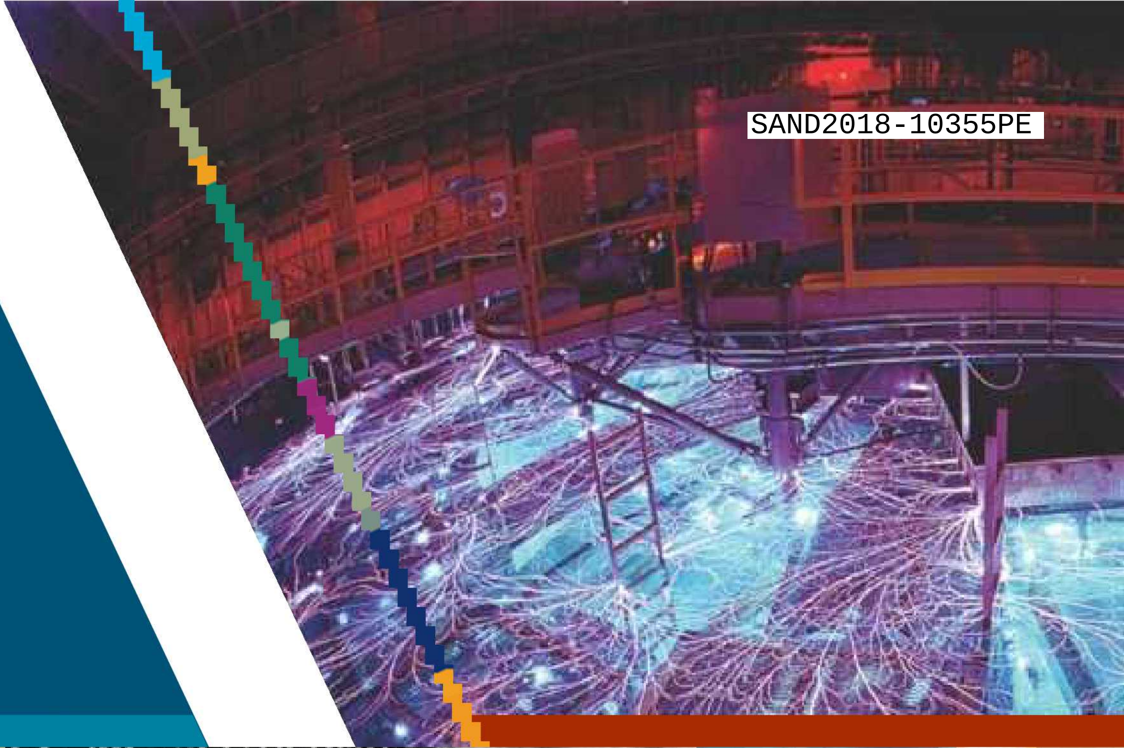


Exceptional service in the national interest

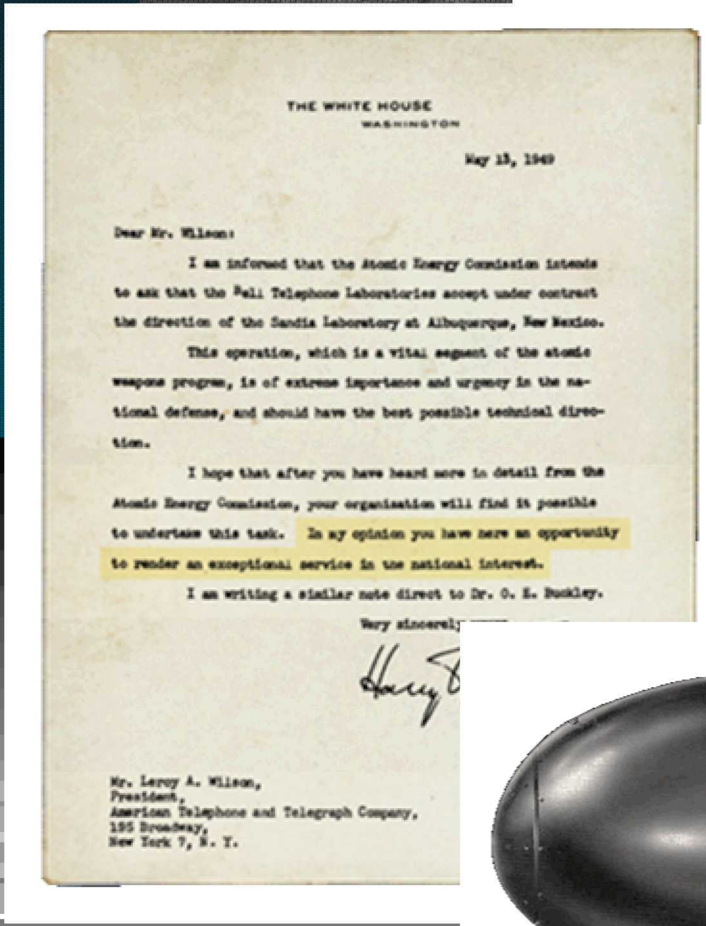
Sandia Statistical Sciences – *Providing innovative statistical solutions for the most challenging national security problems*

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
SAND 2018-4900 PE

SANDIA'S HISTORY IS TRACED TO THE MANHATTAN PROJECT

…In my opinion you have here an opportunity to render an exceptional service in the national interest.

- July 1945
  Los Alamos creates Z Division
- Nonnuclear component engineering
- November 1, 1949
  Sandia Laboratory established
- AT&T: 1949–1993
- Martin Marietta: 1993–1995
- Lockheed Martin: 1995–2017
- Honeywell: 2017–present



THE WHITE HOUSE
WASHINGTON

May 13, 1949

Dear Mr. Wilson:

I am informed that the Atomic Energy Commission intends to ask that the Bell Telephone Laboratories accept under contract the direction of the Sandia Laboratory at Albuquerque, New Mexico.

This operation, which is a vital segment of the atomic weapons program, is of extreme importance and urgency in the national defense, and should have the best possible technical direction.

I hope that after you have heard more in detail from the Atomic Energy Commission, your organization will find it possible to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.

I am writing a similar note direct to Dr. O. E. Buckley.

Very sincerely

Mr. Leroy A. Wilson,
President,
American Telephone and Telegraph Company,
195 Broadway,
New York 7, N. Y.

PURPOSE STATEMENT DEFINES WHAT WE DO

Sandia develops advanced technologies to ensure global peace

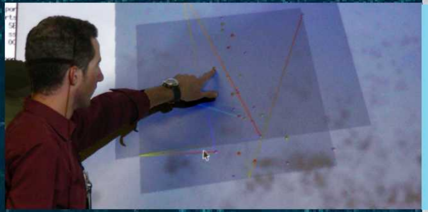
Fulfilling Our National Security Mission

Nuclear Deterrence

Defense Nuclear Nonproliferation

National Security Programs

Energy & Homeland Security



Advanced Science & Technology

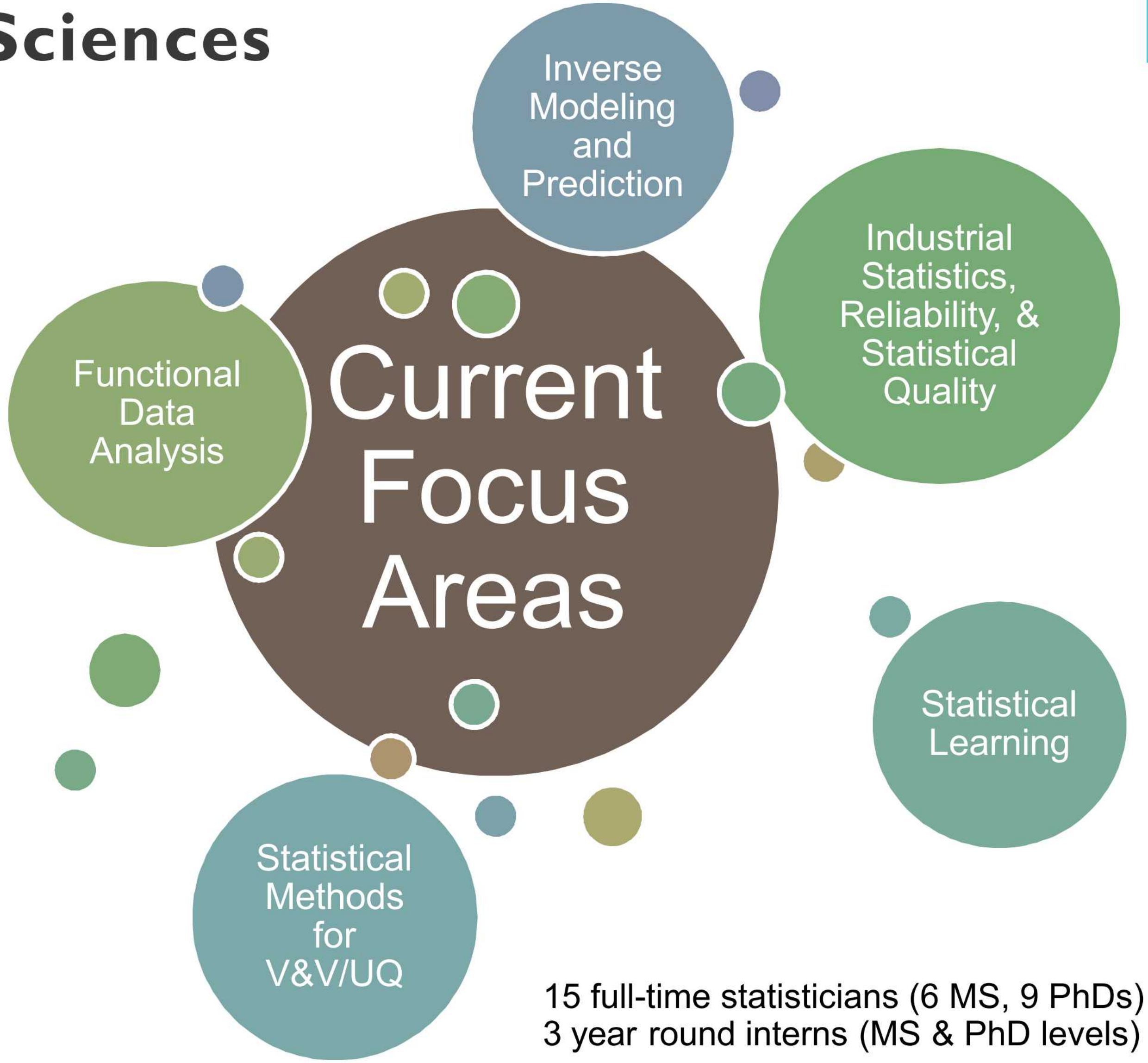
[illegible] of life.

Department of Statistical Sciences

We provide innovative statistical solutions to help solve the most challenging national security problems and are leaders in the advancement of statistical methodologies for national defense applications.

Through research, collaboration, and education we inform the collection, analysis, and interpretation of data to help Sandia execute its missions.

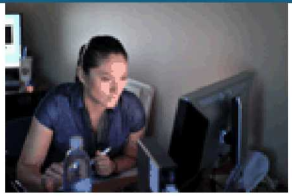
We develop, and deploy statistical algorithms to significantly enhance national security capabilities.

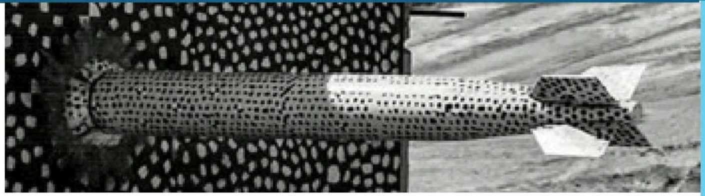


15 full-time statisticians (6 MS, 9 PhDs)
3 year round interns (MS & PhD levels)

Statistics is a foundational capability for all Sandia programs

Statistics & Pre-detonation Nuclear Forensics at Sandia





PRESENTED BY

John R. Lewis Ph.D.

Statistical Sciences

9/19/2018 – Georgia Tech ISyE

Outline

Pre-detonation Nuclear Forensics

Inverse Prediction

1. Down-selecting a useful set of responses
2. How good are our predictions?
3. Utilizing Distributional and Functional Measurements

Review

Future Work

Other Applications

References/Collaborators

Pre-Detonation Nuclear Forensics

Use measurements (Physical, chemical,…) of interdicted nuclear material to infer processing history and origin of the material.

Fig. 1 Sample of uranium–plutonium mixed oxide powder seized in Munich (Germany) in 1994.

Fig. 2 Sample of yellow cake, containing natural uranium, seized in Rotterdam (NL) in 2003.

Mayer, K., Wallenius, M., & Ray, I. (2005). Nuclear forensics—a methodology providing clues on the origin of illicitly trafficked nuclear materials. *Analyst*, *130*(4), 433-441.

The goal is easy to understand….

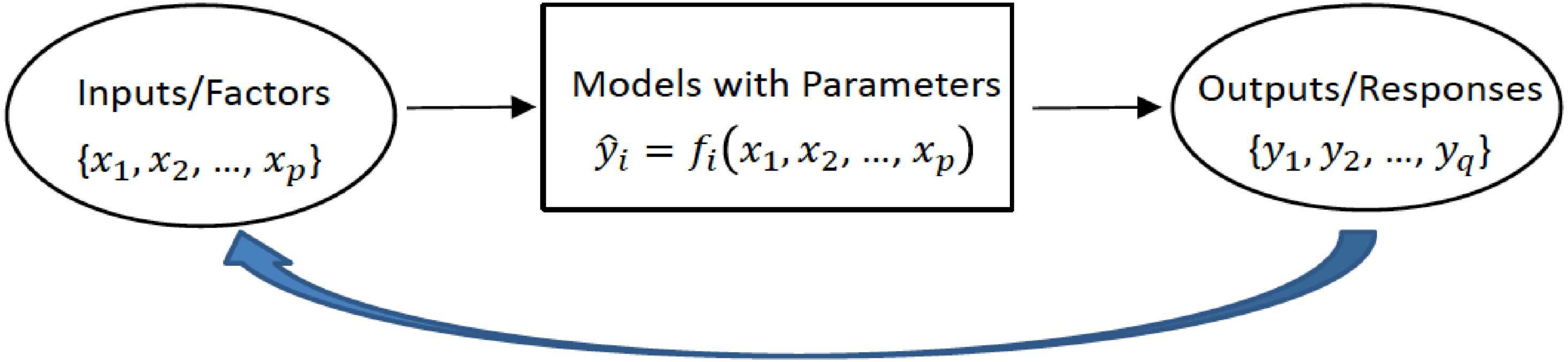
Use measurements taken from interdicted nuclear material to infer processing history and origin of the material.

This Talk

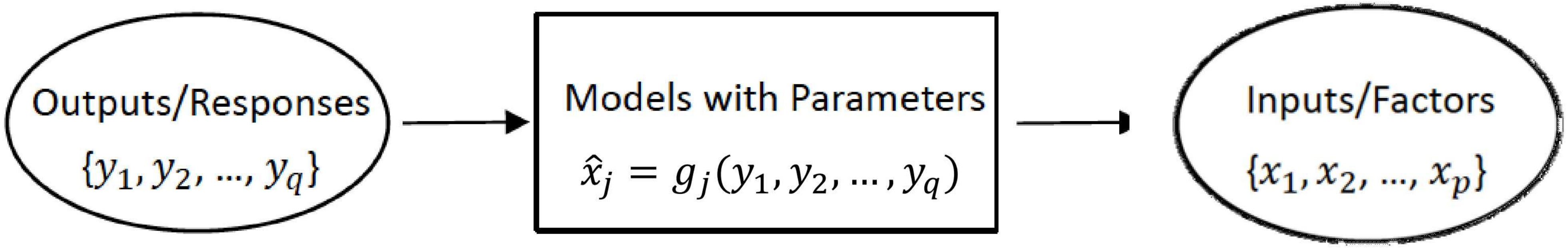
Some of the statistical complexities we have run into and how we have addressed **some** of them so far.

Translating the goal to statistics: 'Inverse Prediction'

Forward/Causal Modeling Approach



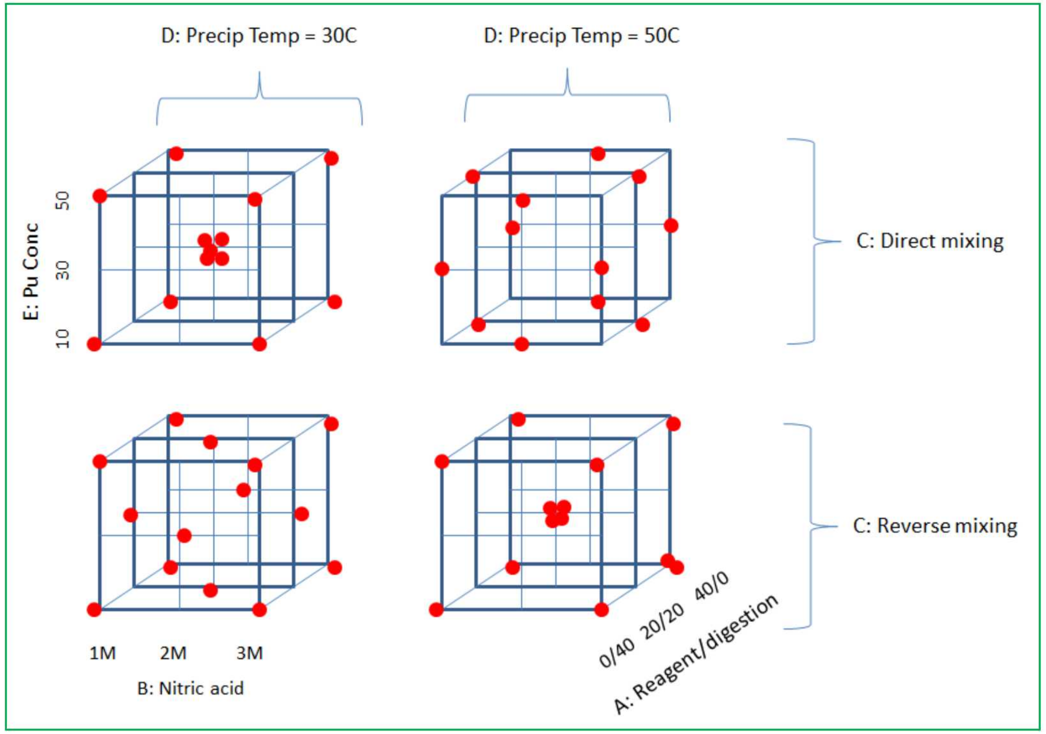
Direct Inverse Modeling Approach



Forward/Causal Modeling

Often a consequence of controlled experiments

Oxalate feed in solution at 0.9M



Example of **part** of a controlled experiment for producing small specimens of Pu(III) oxalate. I-optimality used to design the experiment. Production done at PNNL.

Experimenter identifies

- Factors to be predicted
- Response variables to measure

Experimental design affects

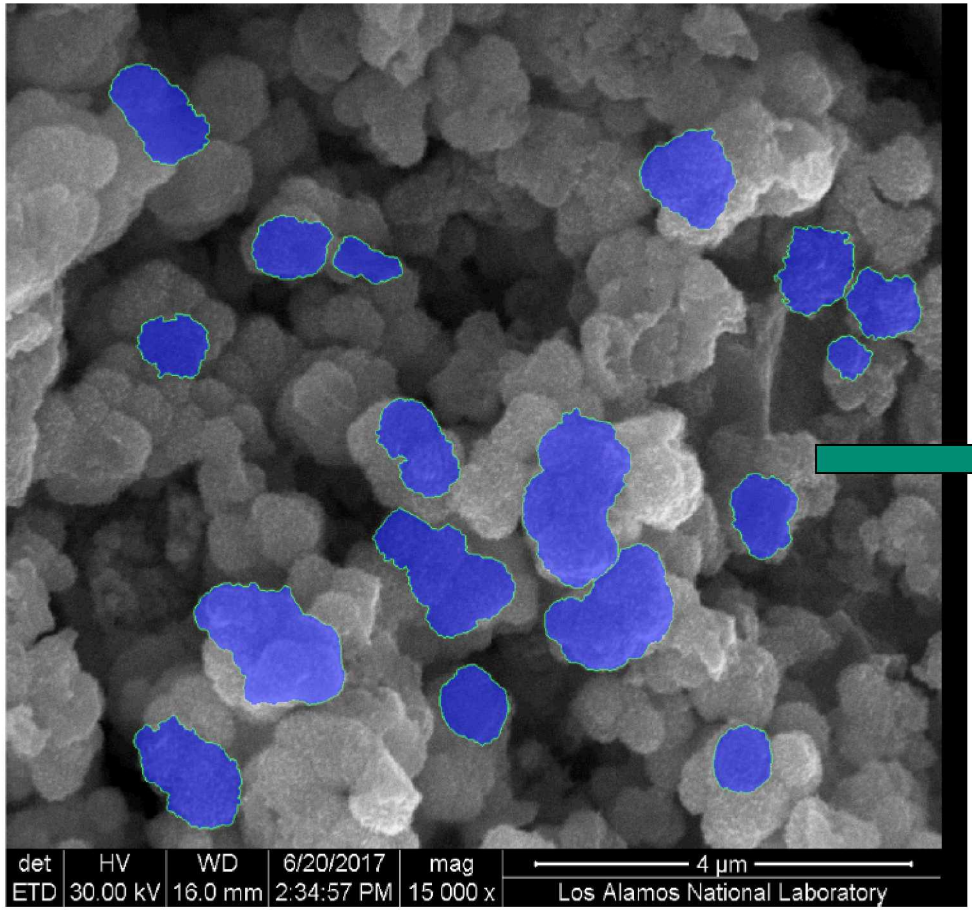
- Relationships that can be model
- Precision of model parameter estimates

Models can be

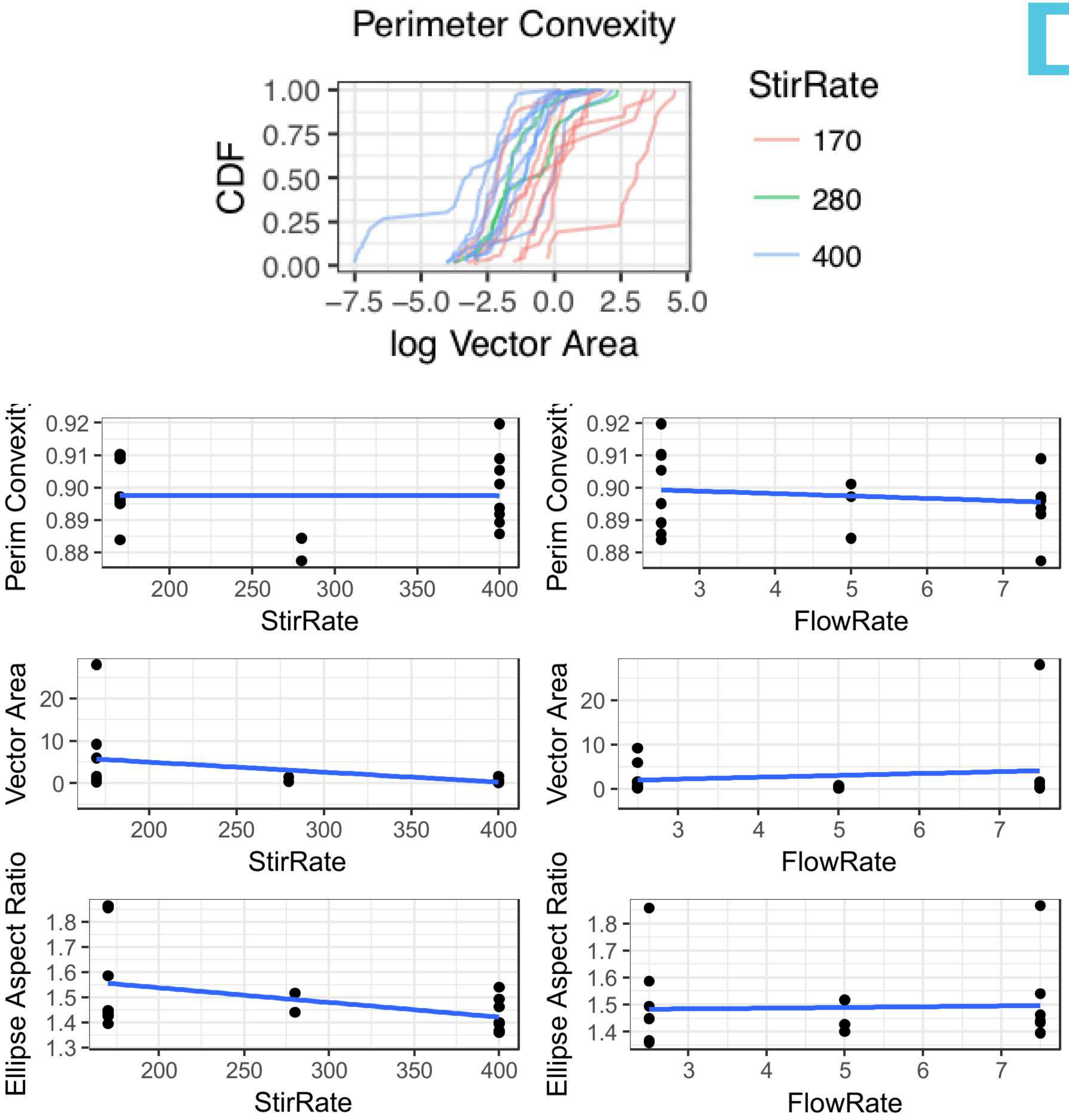
- Science based
- Empirical – e.g. 2nd order response surface models

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{11} X_1^2 + \beta_{22} X_2^2 + \beta_{12} X_1 X_2 + \epsilon$$

Example Measurements



Scanning electron microscope (SEM) image of produced material with particle segmentation



Responses can be distributional, functional, scalar.
Initially, distributional responses were reduced to scalars by

I. Down-Selecting Responses

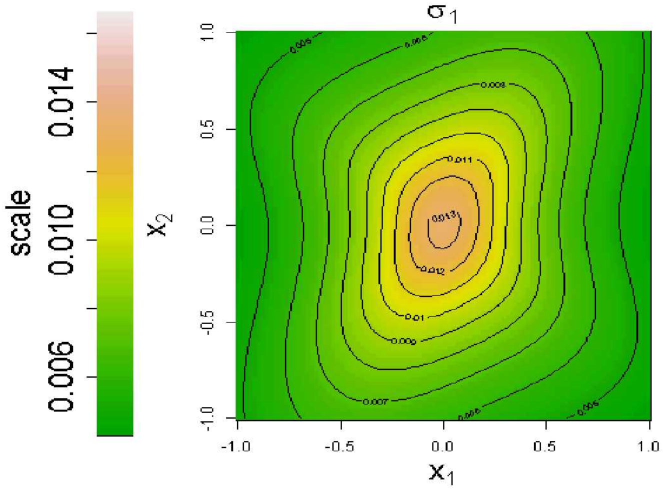
Many responses to be measured

1. Build forward models for each.
2. Invert the forward models to predict processing conditions.

What about interdicted material?

1. Material is limited (amount that will be available unknown).
2. Some measurements are destructive.

$S = \{1, 2, \ldots, 16\}$



Prediction uncertainty of x_1

How do we down-select from candidate responses and associated forward models?

Inferring p-dimensional $\boldsymbol{x}^*$ from q-dimensional $\boldsymbol{y}^*$

Measured Responses

$$\boldsymbol{y}^* = \{y_i^* = f_i(\boldsymbol{\beta}_i; \boldsymbol{x}^*) + \varepsilon_i^*, i = 1{:}\,q\}$$

Predicted Responses

$$\hat{\boldsymbol{y}}^* = \{\hat{y}_i^* = f_i(\widehat{\boldsymbol{\beta}}_i; \widehat{\boldsymbol{x}}), i = 1{:}\,q\}$$

Differences between predicted and measured responses

$$d_i = \hat{y}_i^* - y_i^* = \underbrace{\left[f_i(\widehat{\boldsymbol{\beta}}_i; \widehat{\boldsymbol{x}}) - f_i(\boldsymbol{\beta}_i; \widehat{\boldsymbol{x}})\right]}_{\lambda_i} + \underbrace{\left[f_i(\boldsymbol{\beta}_i; \widehat{\boldsymbol{x}}) - f_i(\boldsymbol{\beta}_i; \boldsymbol{x}^*)\right]}_{\omega_i} - \varepsilon_i^*$$

$$\boldsymbol{d} = \left(d_1, d_2, \dots, d_q\right)^T$$

$$\boldsymbol{V} = Cov(\boldsymbol{d}) = \boldsymbol{V}_{\boldsymbol{\varepsilon}} + \boldsymbol{V}_{\boldsymbol{\lambda}}(\widehat{\boldsymbol{x}}) + \boldsymbol{V}_{\boldsymbol{\omega}}(\widehat{\boldsymbol{x}}) + \cdots$$

One solution (least squares) is $\widehat{\boldsymbol{x}}^* = \underset{\widehat{\boldsymbol{x}}}{arg\ min}\ \boldsymbol{d}^T\, \widehat{\boldsymbol{V}}(\widehat{\boldsymbol{x}})^{-1}\boldsymbol{d}$

Covariance of $\hat{x}^*$

Assume $f_i(\beta_i; x)$ are continuous in factors and not highly non-linear

First-order expansion of $f_i(\beta_i; x)$ near x^*

$$E(y_i|x) = f_i(\beta_i; x) \approx f_i(\beta_i;\ x^*) + \sum_{j=1}^{p} J_{ij}(x^*)\left(x_j - x_j^*\right)$$

$$J_{ij}(x^*) = \frac{\partial}{\partial x_j} f_i(\beta_i; x^*)$$

$$\hat{C}_{\hat{x}^*} = \left(\hat{J}^T(\hat{x}^*)\hat{V}(\hat{x}^*)^{-1}\hat{J}(\hat{x}^*)\right)^{-1}, \text{ where } \hat{J}_{ij}(\hat{x}^*) = \frac{\partial}{\partial x_j} f_i\left(\hat{\beta}_i; \hat{x}^*\right).$$

Estimated Covariance based on local linear regression of $\boldsymbol{y}^*$ on $\hat{J}_{ij}$

In a neighborhood of $\hat{x}^*$, multivariate response is

- **Informative** if diagonal elements of $\hat{C}_{\hat{x}^*}$ are sufficiently small
- **Discriminating** if the off diagonal elements of $\hat{C}_{\hat{x}^*}$ are sufficiently small

Down-Selection of a Multivariate Response

1. Consider possible subsets of responses – each has its own forward model
2. Evaluate $\hat{C}_{\hat{x}^*}$ for each subset
   - Done over a region of interest of the input space
3. Select a subset that is adequate in terms of being informative and discriminating

Example: CON-2 Glass*

Goals:

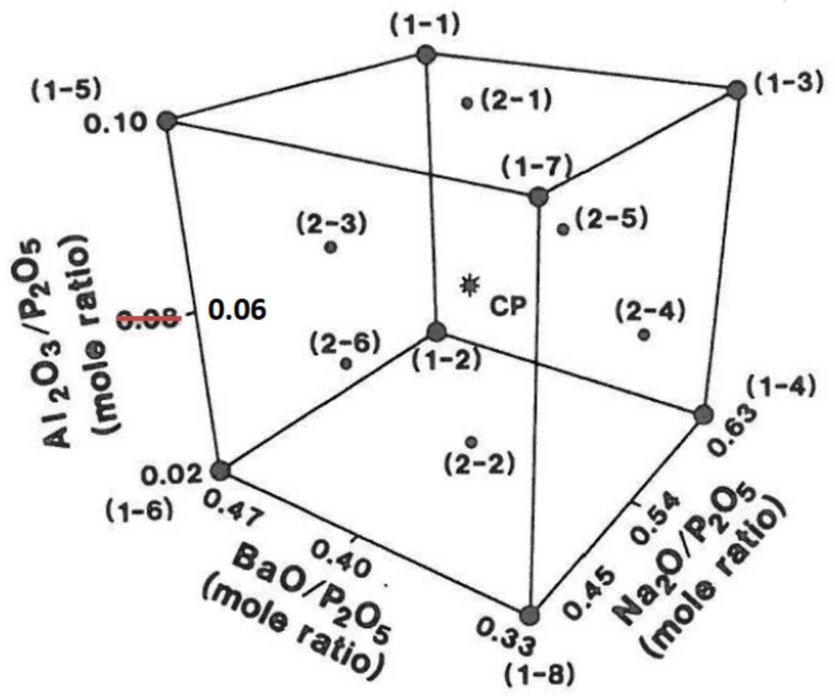
- Understand effects of compositional variation on physical properties of the glass (forward models)
- Predict composition from physical properties (inverse prediction)

Factors: 3 mole ratios:

$$x_1 = \frac{Na_2O}{P_2O_5}, x_2 = \frac{BaO}{P_2O_5}, \quad x_3 = \frac{Al_2O_3}{P_2O_5}$$

Responses: 6 Physical Properties

Targeted Design points (n = 8 + 6+ 3cps)



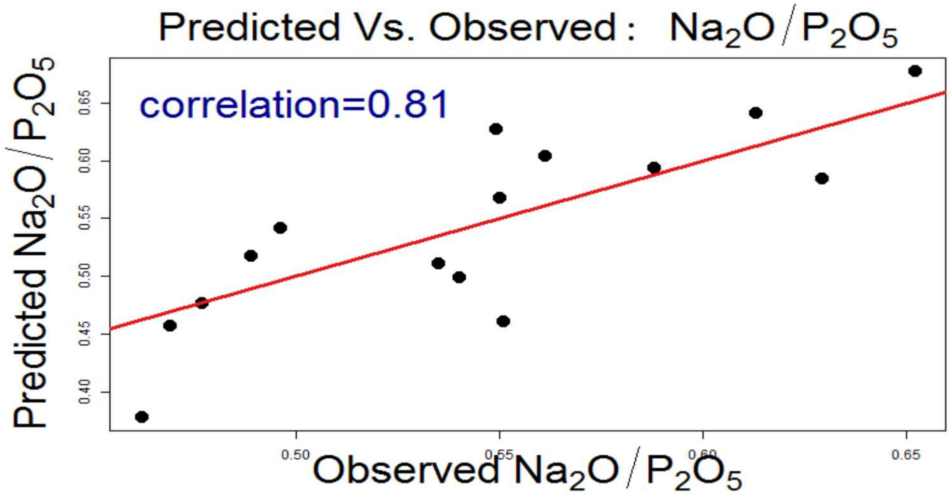
* Compositional Quality Control Study of CON-2 Glass (C. Nelson, E. V. Thomas, and P. R. Wengert), 1986, Sandia National Laboratories Technical Report, SAND86-0430.

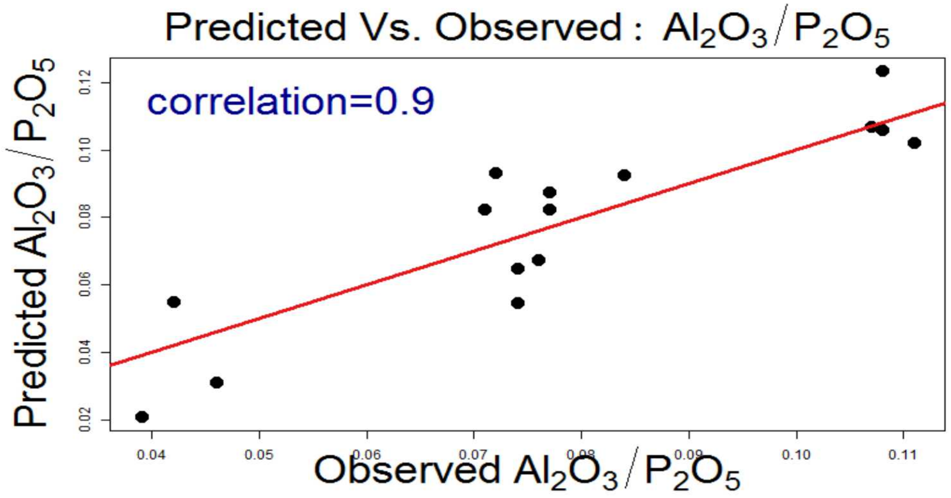
Forward Models – Linear Main Effects Models

$$\hat{Y}_i = \hat{\beta}_{i0} + \hat{\beta}_{i1}X_1 + \hat{\beta}_{i2}X_2 + \hat{\beta}_{i3}X_3$$

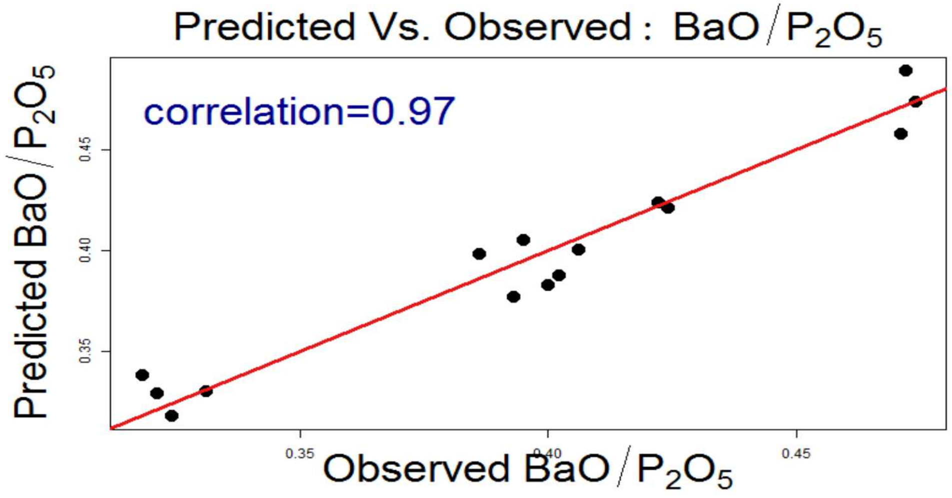
Property: $i = 1, \ldots, 6$	$\hat{\beta}_0$	$\hat{\beta}_1\ (Na_2O)$	$\hat{\beta}_2\ (Ba0)$	$\hat{\beta}_3\ (Al_2O_3)$	$\hat{\sigma}_\varepsilon$	R^2
1. Coeff. of Thermal Exp. (α)	155.8 (6.1)	70.59(10.3)	----	-216.5(31)	3.12	0.86
2. Softening Temp. (T_s)	392.7(15.5)	-104.7(24.6)	----	694.6(63)	5.73	0.93
3. Glass Transition Temp. (T_g)	374.8(14.7)	-104.5(23.7)	----	412.1(66)	6.39	0.82
4. Crystallization Temp. (T_x)	570.5(28.9)	-219.5(48.5)	----	709.8(147)	14.7	0.74
5. Density (ρ)	2.534(0.022)	----	1.113(0.051)	0.484(0.119)	0.0119	0.97
6. Index of Refraction (n)	1.498(0.003)	0.0097(0.004)	0.0834(0.005)	0.1036(0.0123)	0.00113	0.97

Inverse Predictions Using All Responses





Red line: y = x



Multivariate response good for predicting BaO and Al_2O_3, not as good for Na_2O

- Strongest models don't depend heavily on Na_2O
- Intuition: need strong forward models for inverse prediction

Comparing ‘Informativeness’ of Different Subsets of Responses

$$\hat{C}_{\hat{X}^*} = \left(\hat{J}^T(\hat{X}^*)\widehat{V_\epsilon}^{-1}\hat{J}(\hat{X}^*)\right)^{-1}$$

Subset	σ_1 (Na_2O)	σ_2 (BaO)	σ_3 (Al_2O_3)
All Responses	0.08	0.013	0.018
w/o α	0.11	0.014	0.02
w/o T_s	0.14	0.024	.037
w/o ρ	0.08	0.02	0.019

Good predictive ability for BaO and Al_2O_3

Significant increases in prediction variance for

- Na_2O when excluding α and T_s
- BaO when excluding T_s and ρ
- $Al_2O_3$3 when excluding T_s

Considering 'Discriminating' Ability

For Main Effects Forward Models: $\hat{J}_{ij}(\hat{x}^*) = \hat{\beta}_{ij}$

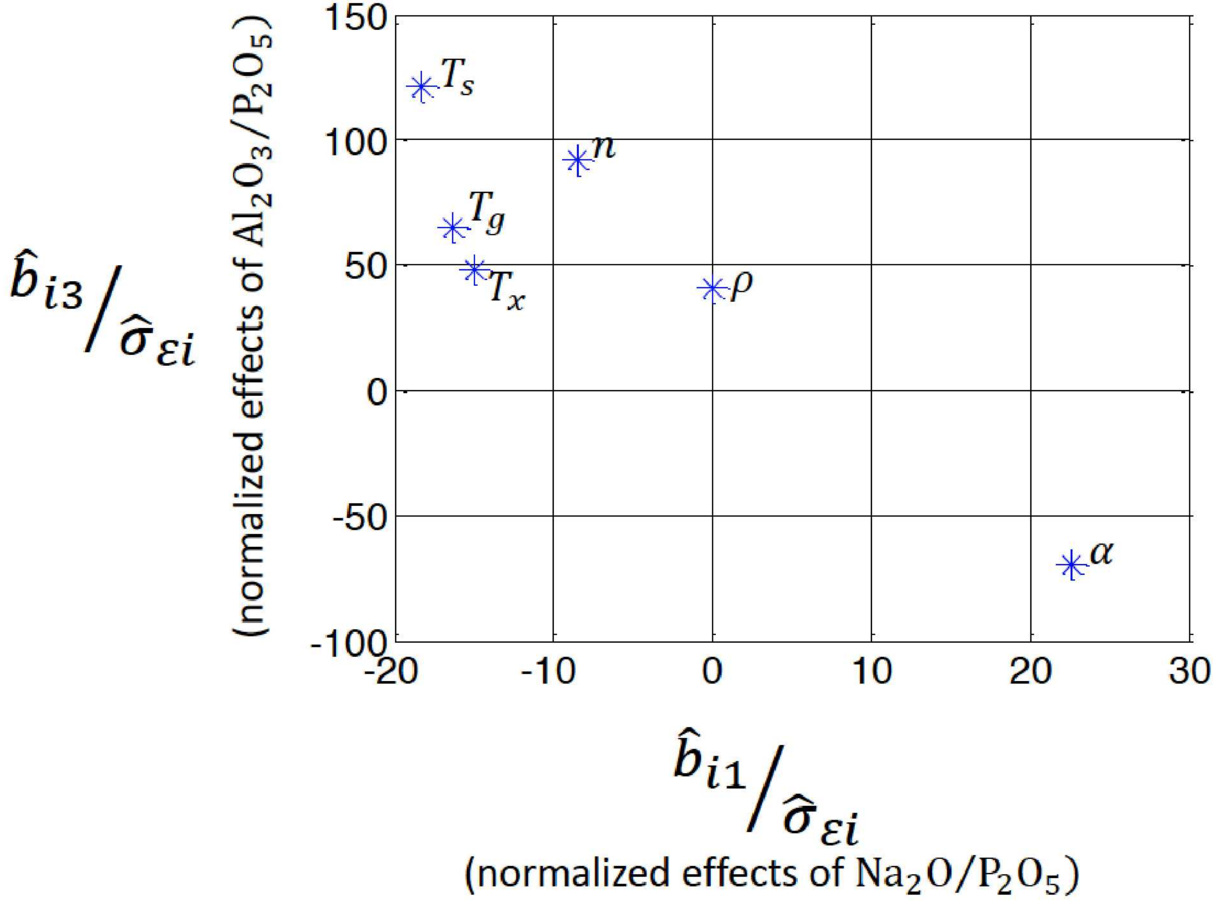
Assume: $\hat{V} = \hat{V}_\epsilon = \mathrm{diag}(\hat{\sigma}_i^2, i = 1, 2, \ldots, 6)$

$$\hat{C}_{\hat{x}^*} = \left(\hat{J}^T(\hat{x}^*)\hat{V}^{-1}\hat{J}(\hat{x}^*)\right)^{-1} = \left(\hat{B}^\top \hat{V}^{-1}\hat{B}\right)^{-1}$$

High correlation indicates responses not discriminating.

Prediction errors are correlated.

Displayed by correlation in the columns of $\hat{\boldsymbol{B}}$



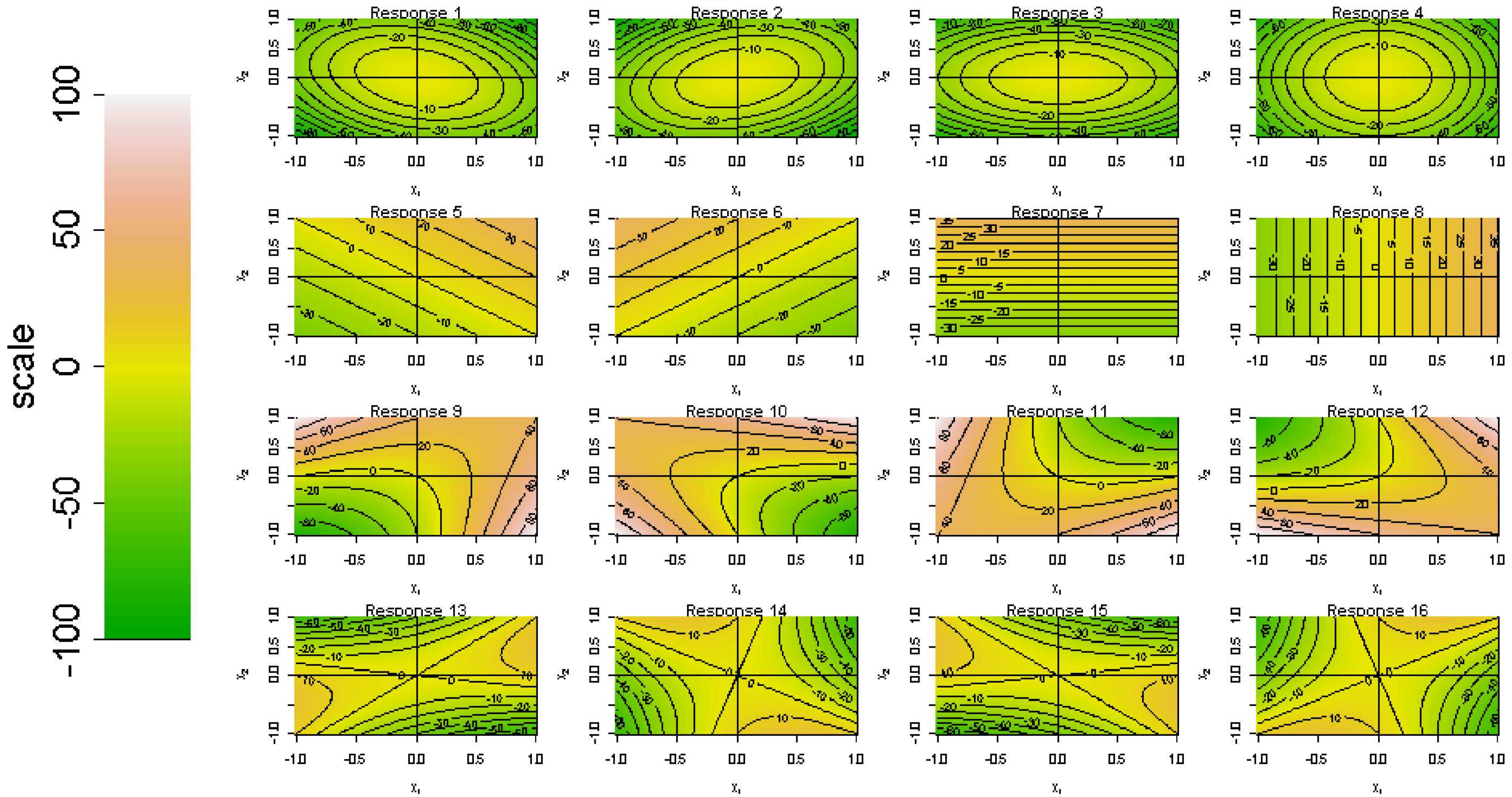
Summary of CON-2 Glass Study

- Responses associated with strong models are useful
- Poor ability to predict Na_2O/P_2O_5
  - Effects of this variable on responses are weak
- Poor ability to discriminate between Na_2O/P_2O_5 and Al_2O_3/P_2O_5
  - Effects are highly correlated
- Good ability to predict BaO/P_2O_5 and Al_2O_3/P_2O_5
  - For BaO/P_2O_5 : Density and T_s are useful and complementary

Further Investigation: 16 Known Response Surfaces

Goal: Choose a subset of the 16 response surfaces that is ***informative*** (small prediction variance) and ***discriminating*** (sufficiently dissimilar shapes) for prediction of x_1 and x_2

16 response surfaces



1-4: peaks

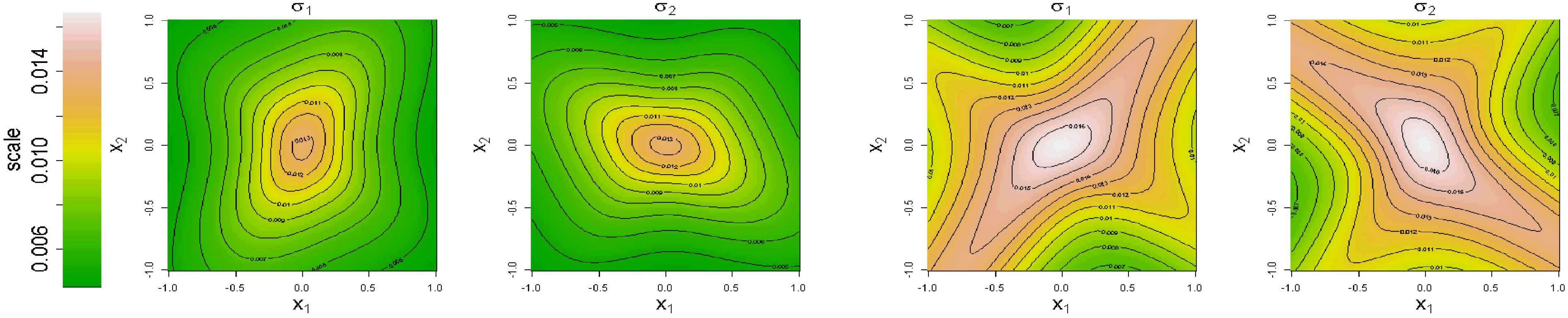
5-8 : hillsides

9-12: rising ridges

13-16: saddles

Prediction St. Dev. Across Design Space

$S = \{1,2,\dots,16\}$ $\quad$ $S = \{9,10,11,12\}$



- Value depends on x^*. Smaller standard deviation across design space when using all 16 responses
- Relative increase using just four responses is small across the design space

Quantifying Differences in Prediction Variance

Subset	$\sqrt{Var_{avg}\ \hat{x}_1^*}$	$\sqrt{Var_{avg}\ \hat{x}_2^*}$
{1,2,…,16}	0.0075	0.0075
{7,8}	0.0286	0.0286
{3,7,9,13}	0.0291	0.0154
{9,10,11,12}	0.0121	0.0121

~ 4x larger (for $\hat{x}_1^*$)

~ 1.6x larger for ¼ of responses

- Set {9,10,11,12} is a good choice if constraints exist in obtaining new measurements
- Responses in this set complement each other well – i.e. steep contours are present in one or more of the responses throughout the range of interest

2. How good are our predictions?

Poor predictions could be due to

- Use of the wrong method, assumptions
- Missing responses/factors
  - Can choose to analyze material in many ways
- Calibration data not informative
  - Unknown history of material interdicted in the future
  - Unknown, uncontrolled factors.

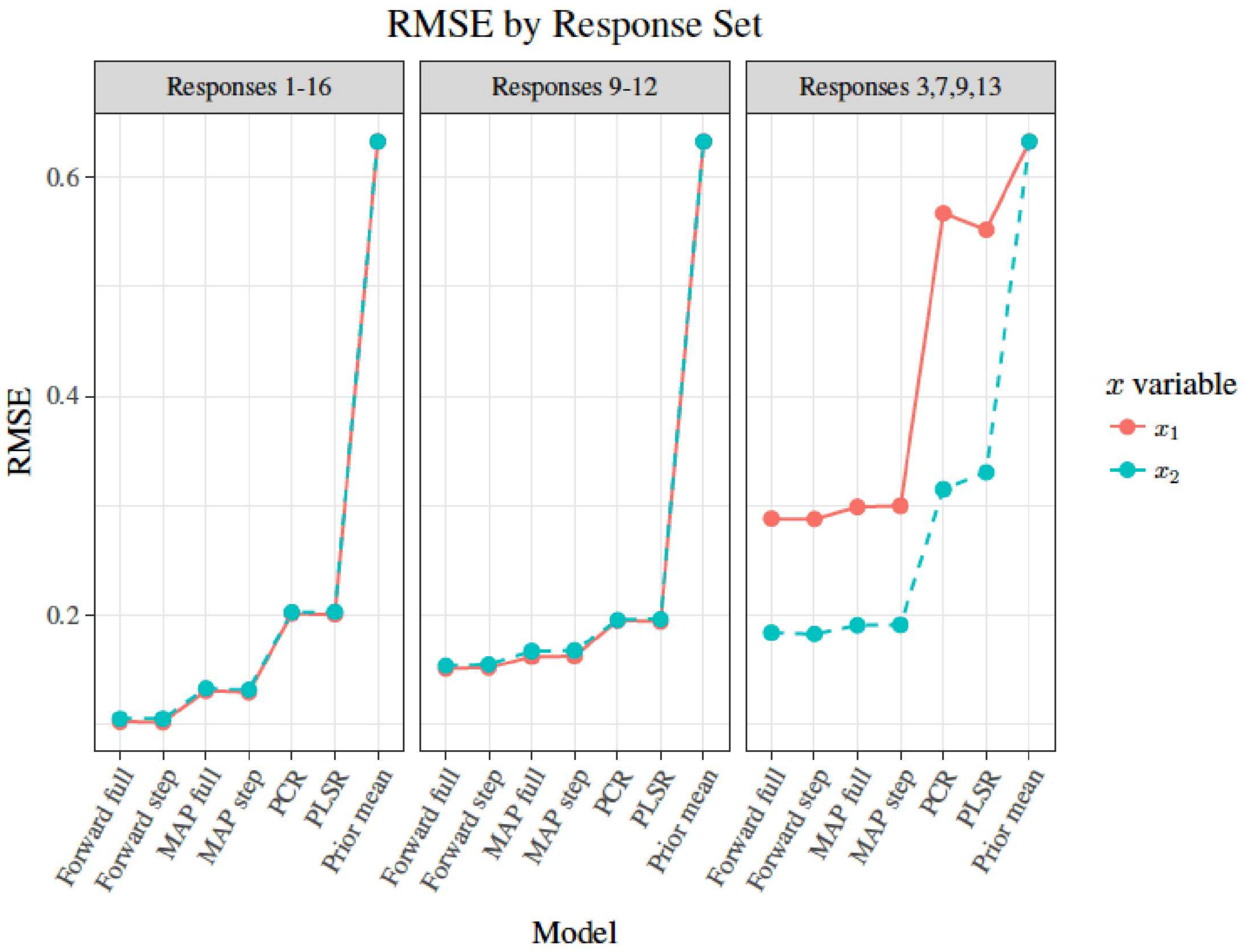
A Pragmatic Approach

- Use several methods to predict source characteristics x
- Assess the level of consistency across the different predictions
- Consult with subject matter experts

- **Consistency provides confidence**
  - Robustness to the different assumptions
  - Only marginal gains from additional responses or methods
- **Lack of consistency must be investigated:**
  - Why do certain methods fail?
  - Any additional responses available?

Example using the 16 Response Surfaces

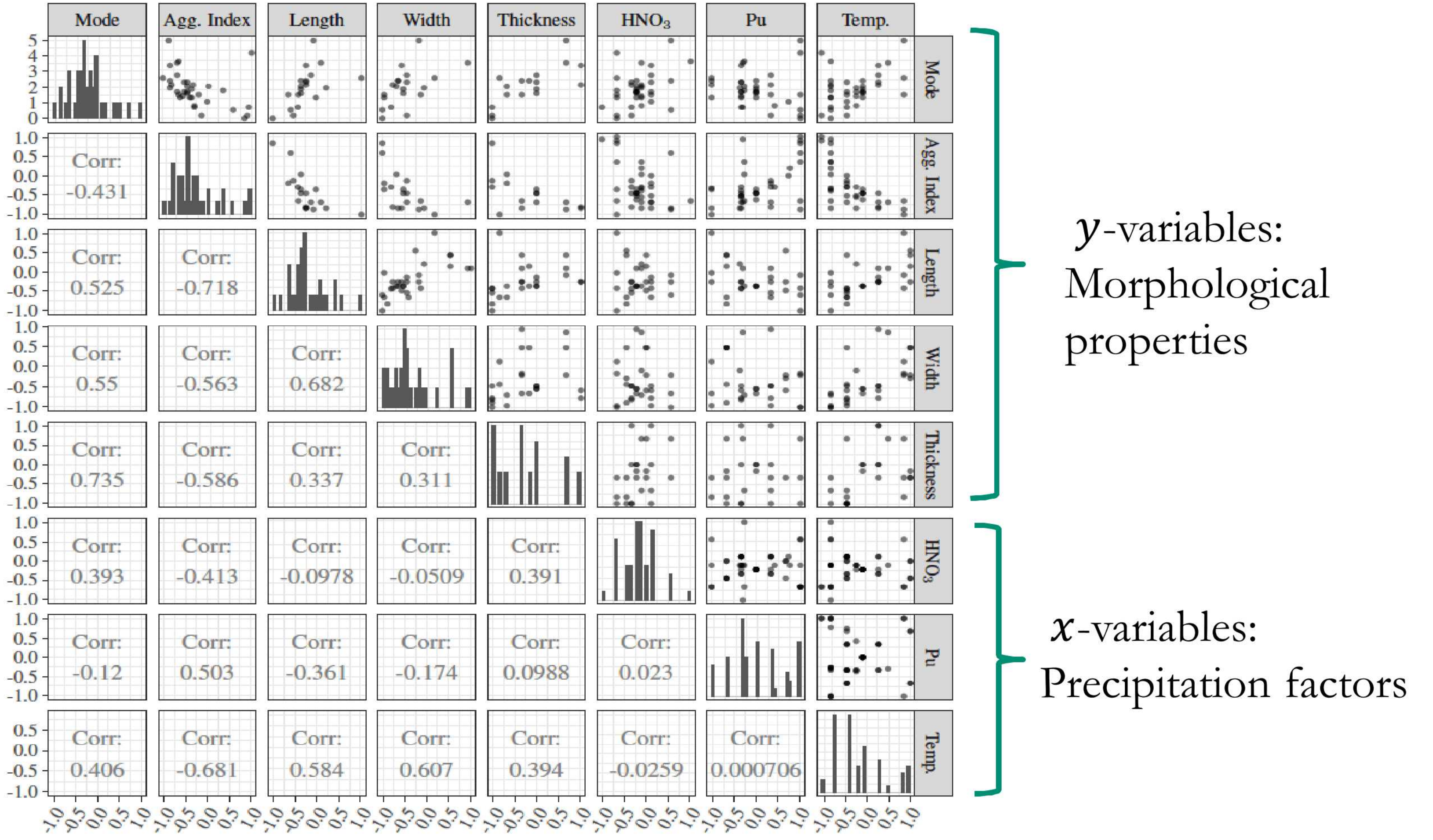
- Simulation:
  - Training data on 3x3 grid
  - Test data on 11x11 grid
  - Make predictions, compute RMSE
- Methods:
  - Forward Models: linear models (freq./Bayes)
  - Direct Inverse Models: PCR, PLSR
  - Prior Mean – predict the center point (a reference)
- If given just responses 3,7,9,13:
  - Large variability
  - Evidence that more responses are needed



Average RMSE across 100 simulated data sets for each method and three sets of responses.

Pu(III) Oxalate Precipitation Data*

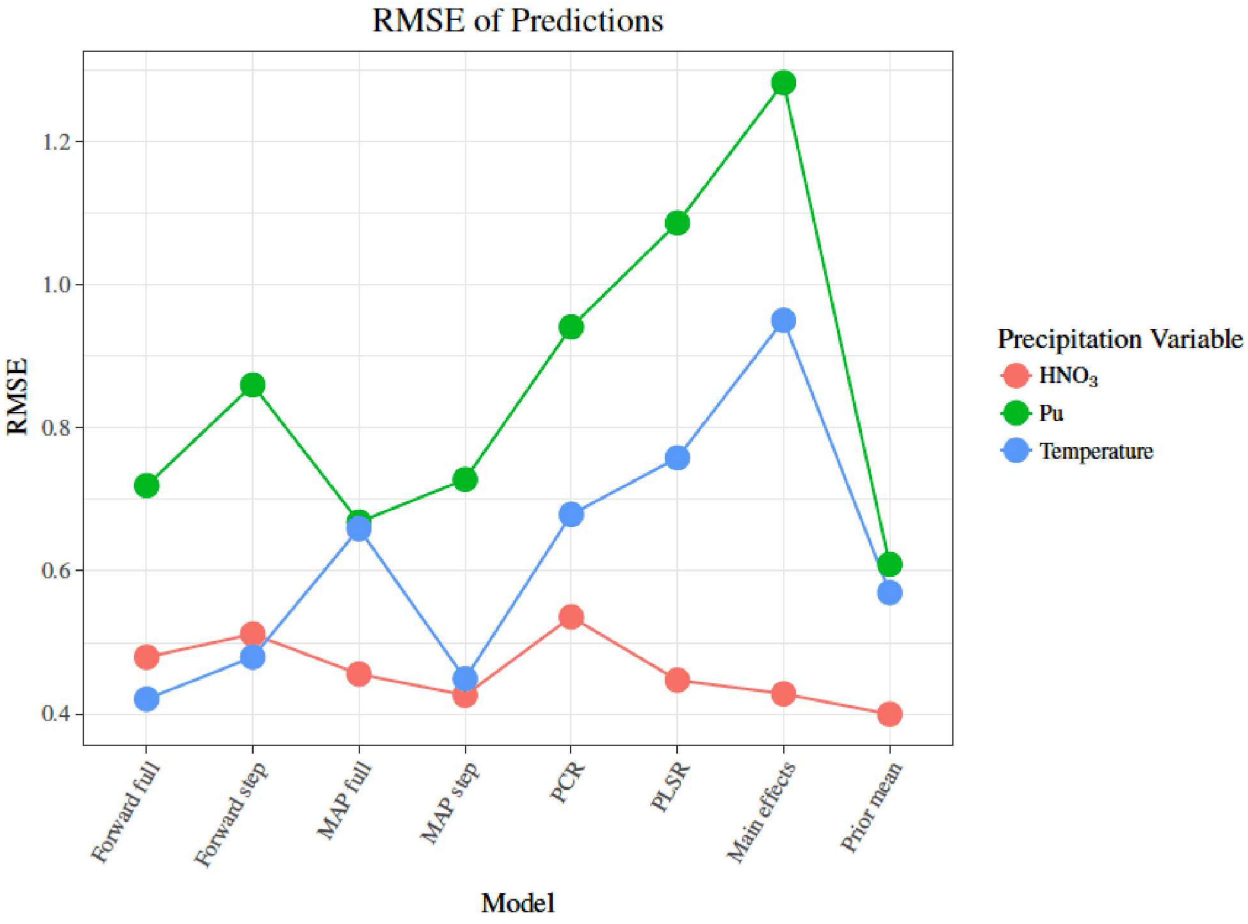
Characterize effects of precipitation factors on morphological properties of calcined Pu powder



Are the available set of morphological properties predictive of the precipitation factors?

* G. A. Burney, P. K. Smith, Controlled puo2 particle size from Pu(III) oxalate precipitation, Tech. rep., Savannah River Laboratory Technical Report DP-1689 (1984).

Overall - No



Average RMSE over LOOCV sets for several prediction methods. The prior mean results are on the right an act as a baseline.

- Weak relationships between responses and processing conditions
- Prior mean (i.e. predicting center of the design space does comparatively well)
- 'Best' method is inconsistent for the precipitation factors.
- Large differences exist between similar methods

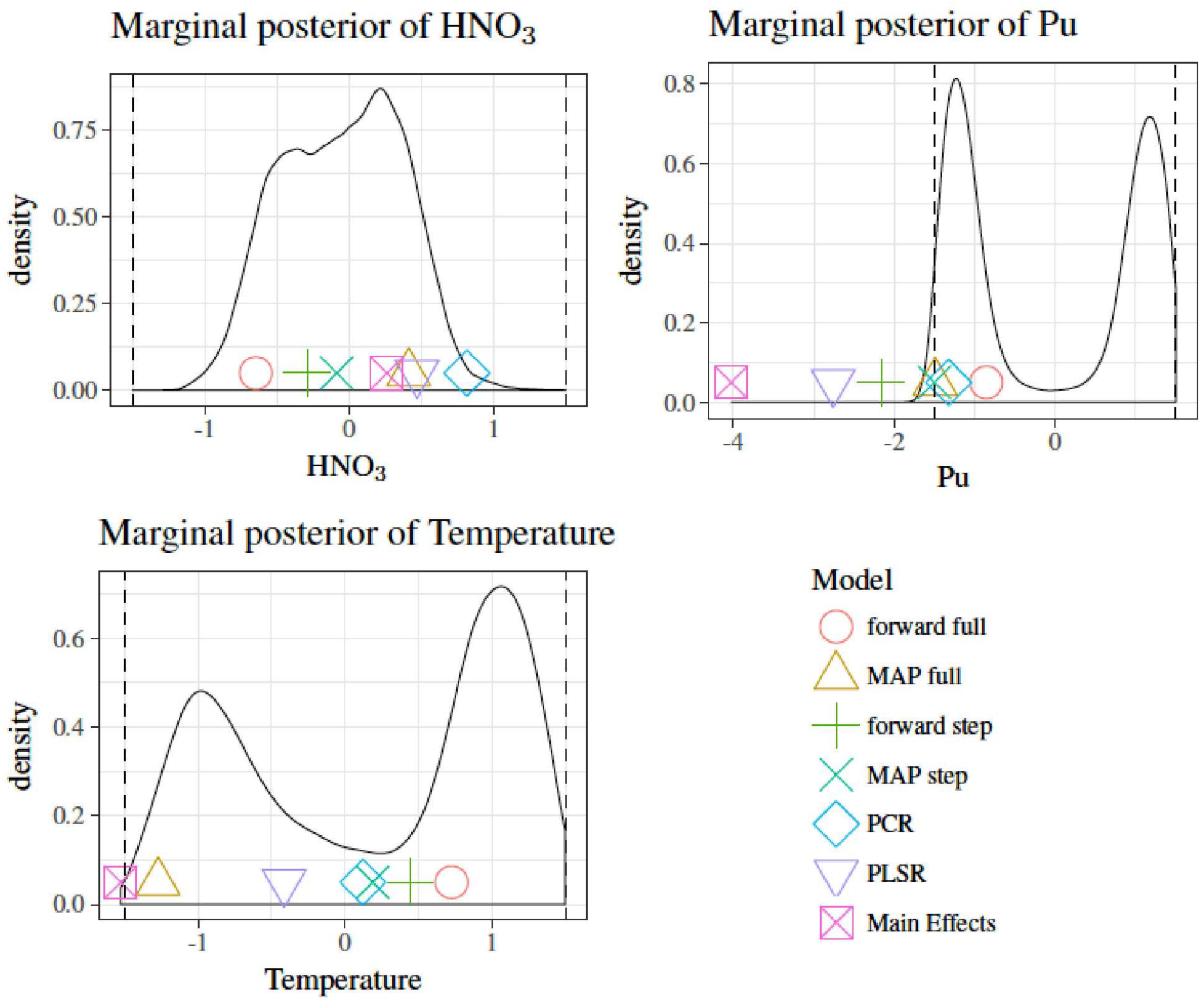
Inconsistent Predictions – Ambiguous ‘Best Estimates’

Indicated by

- Multimodal Posteriors
- Inconsistent predictions across methods

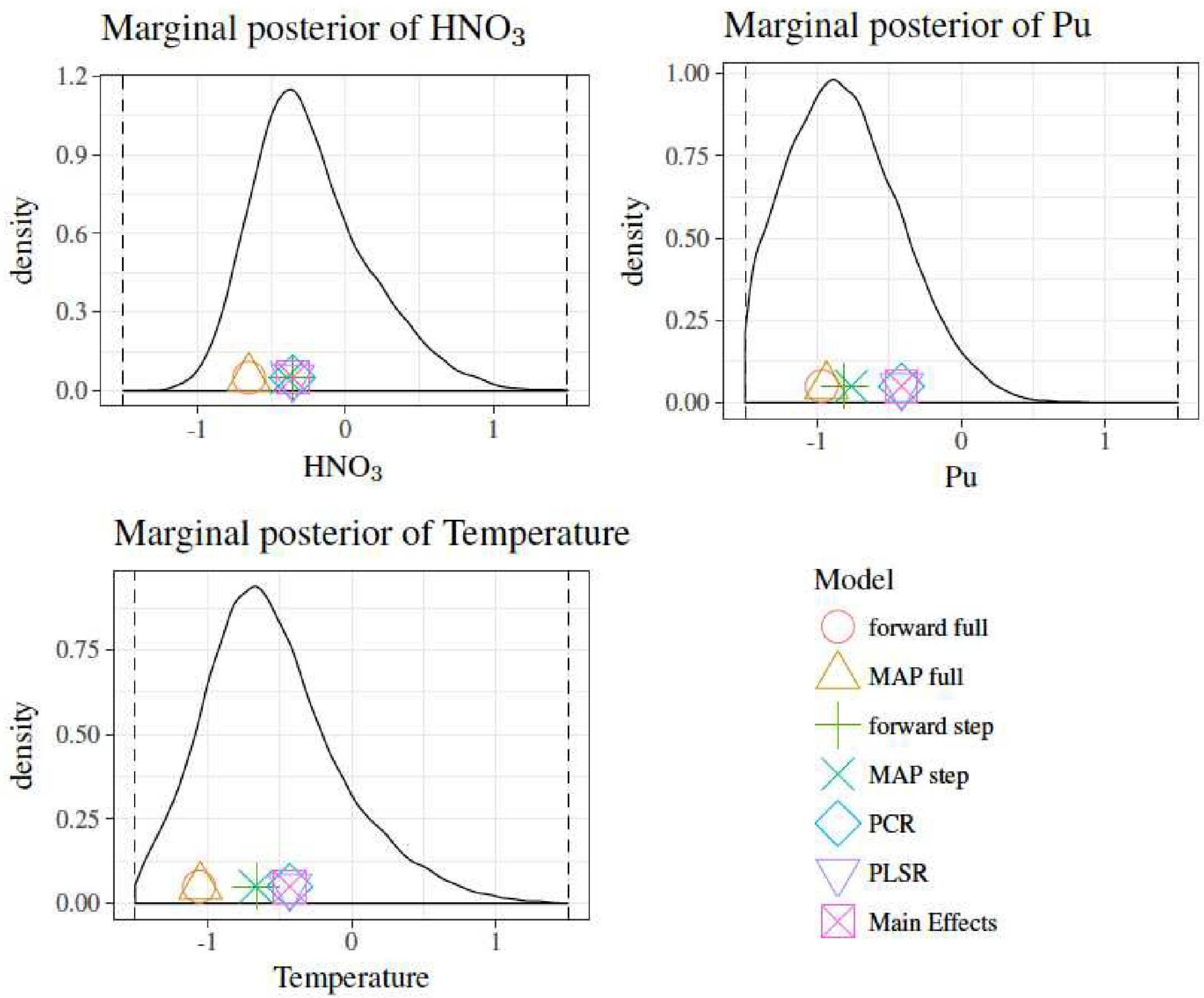
Likelihood for full-Bayesian model adds unknown x^* to set of parameters

$$\mathcal{L}(\boldsymbol{\theta}|\boldsymbol{y}) = \left(\prod_{j=1}^{q} \mathcal{L}_j(\theta_j, \sigma_j|\boldsymbol{y_j})\right)\left(\prod_{j=1}^{q} f_j(y_j^*|X^*, \theta_j, \sigma_j)\right)$$

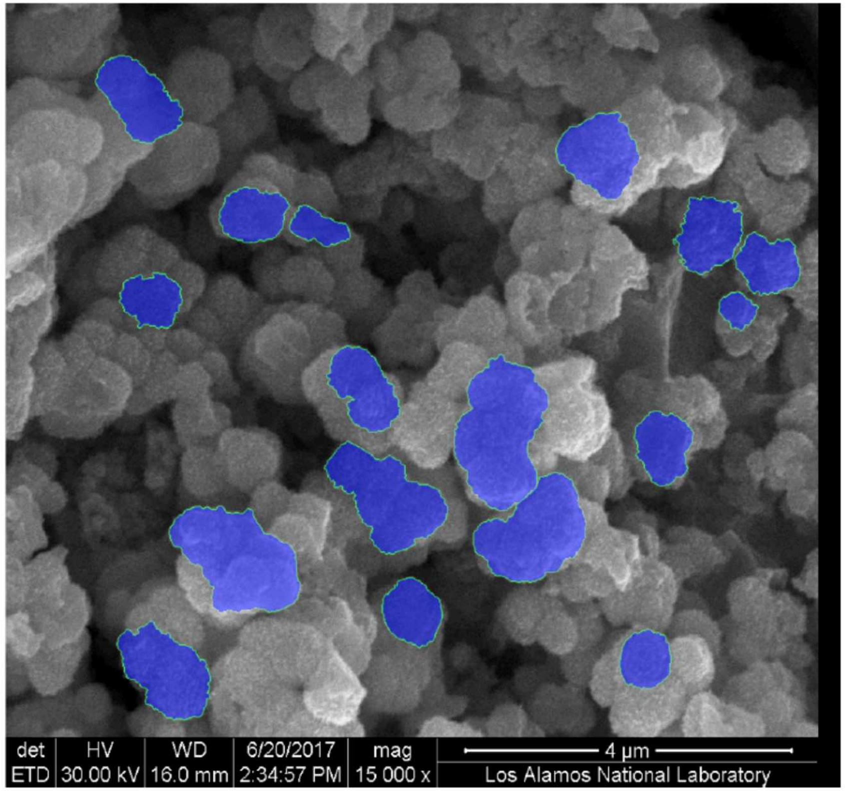


Marginal Posteriors for a single x^* along with predictions under several different methods.

If we had a better set of responses; stronger causal relationships



3. Utilizing Distributional and Functional Measurements



SEM microscope image of powder with particle segmentation

- Image segmentation - distributional measurements
  - Vector Area, Convexity, Circularity, etc.
- Summarized with means and standard deviations

Using the entire distribution?

Inverse Prediction using Functional Regression

Functional Regression Model – Functional response, with scalar covariates

$$W_{ij}(t) = \boldsymbol{X}_j' \boldsymbol{\beta}_i(t) + \epsilon_{ij}(t)$$

$W_{ij}(t)$ - j^{th} observation of the i^{th} functional response variable, indexed by t
$\boldsymbol{\beta}_i(t)$ - i^{th} functional coefficient
X_j - vector of covariates

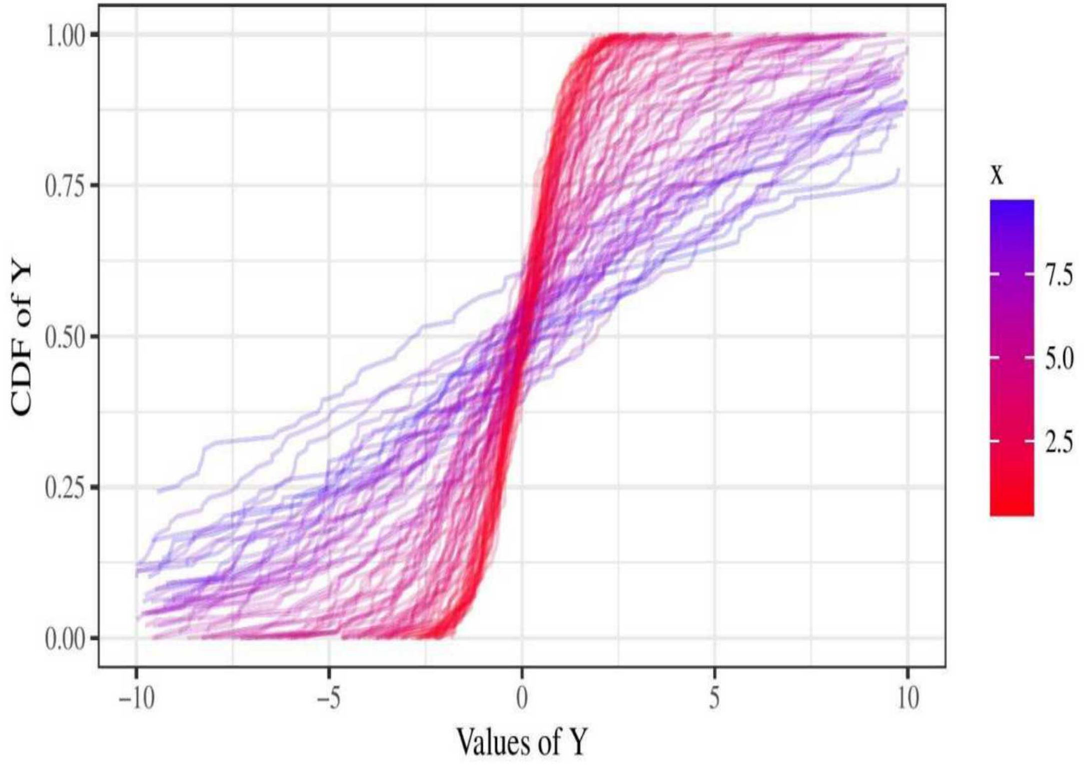
One method for inverse prediction

$$\widehat{\boldsymbol{X}}^* = \arg\min_x \sum_{j=1}^{q} \int \left| \widehat{W_j}(t) - W_j^*(t) \right| dt$$

$W_j^*(t)$ – new set of responses, $\widehat{W_j}(t) = x' \widehat{\boldsymbol{\beta}_j}(t)$

Variants – different loss functions, including functional alignment, Bayesian functional regression, etc.

Simulated Example

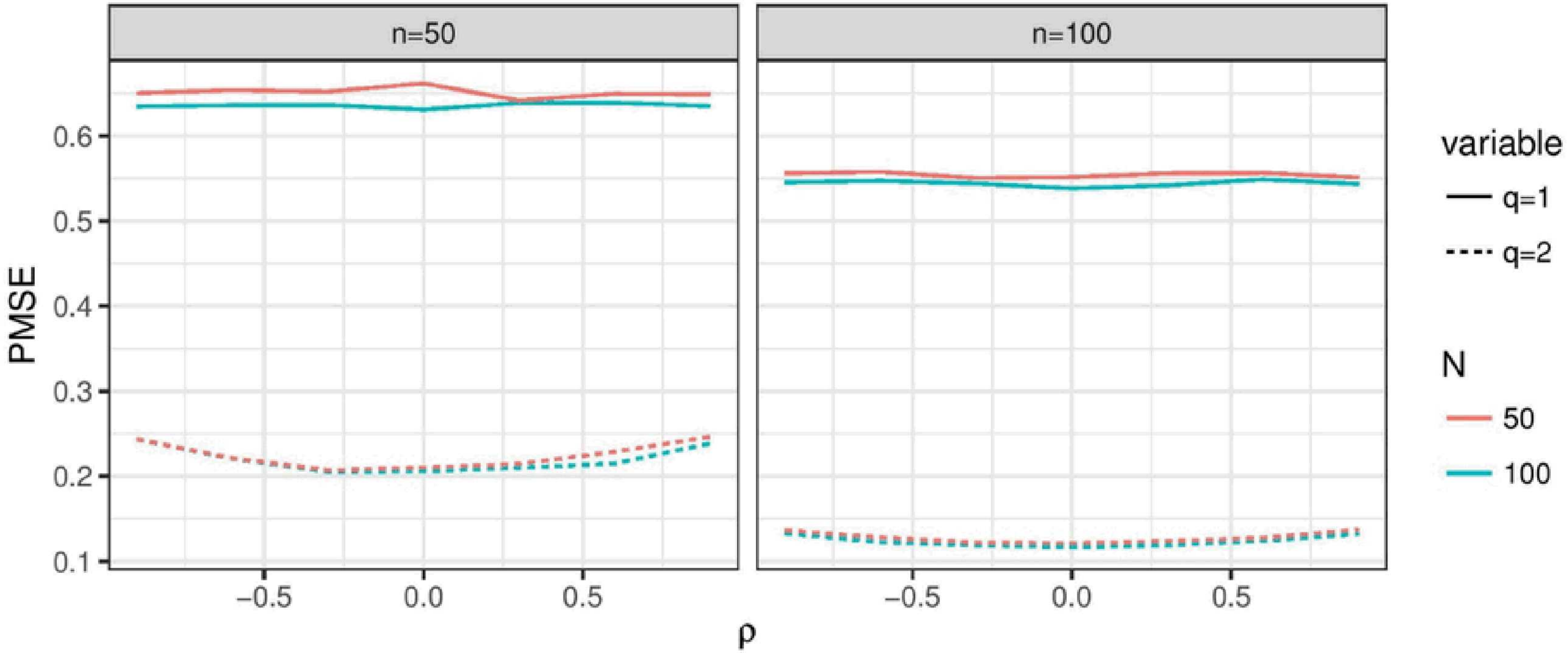


Classic Heteroscedasticity

- All the means are equal – not affected by x
- Could base models on the variance
  - x may not just affect variances
- Use eCDF as a functional response
  - Similar to the data we expect from image segmentation

Simulated Example Con't.

- n - number of experimental trials
- N – number of distributional samples used to estimate CDFs
- q – number of response functions
- ρ – a measure of correlation between the response functions



PMSE of inverse prediction of a test set of x's. Regressions fit to independent training sets varying n, N, q, and ρ.

Analysis with Bench-Scale Uranium Data

- 18 experimental runs
- 5 explanatory variables: UNO_3 ratio, stir rate, flow rate, end pH, and temperature
- 14 distributional responses
- Responses: particle characteristics from image segmentation*
- Correlated responses – use a subset of at most 5

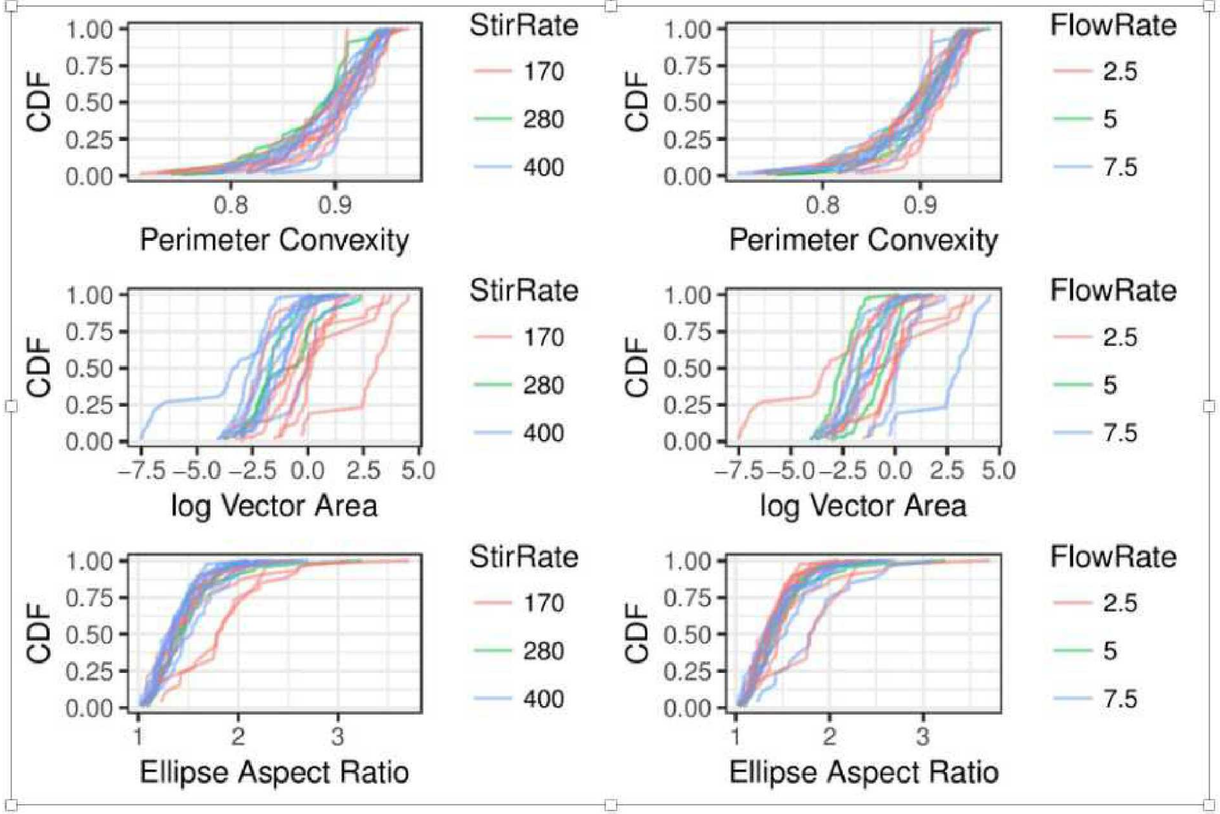


Figure 8. Empirical CDFs for 3 response variables grouped by experimental run colored according to Stir Rate on left and Flow Rate on right. There is noticeable grouping by Stir Rate for log Vector Area while for Flow Rate it looks like a random scatter.

*D. Schwartz. Documentation of operational protocol for the use of mama software. Technical report, Los Alamos Technical Report LA-UR-16-20297, 2016.

Results

	UNO3ratio	StirRate	FlowRate	EndpH	Temp
Standard-5 Y	83.31	135.70	3.67	3.72	19.74
Functional-5 Y	79.35	81.53	3.42	2.65	16.89
Functional-3 Y	84.84	84.28	3.33	2.71	16.64
Functional-1 Y	76.99	85.30	3.37	2.79	16.41

Table: Root PMSE using original scale data.

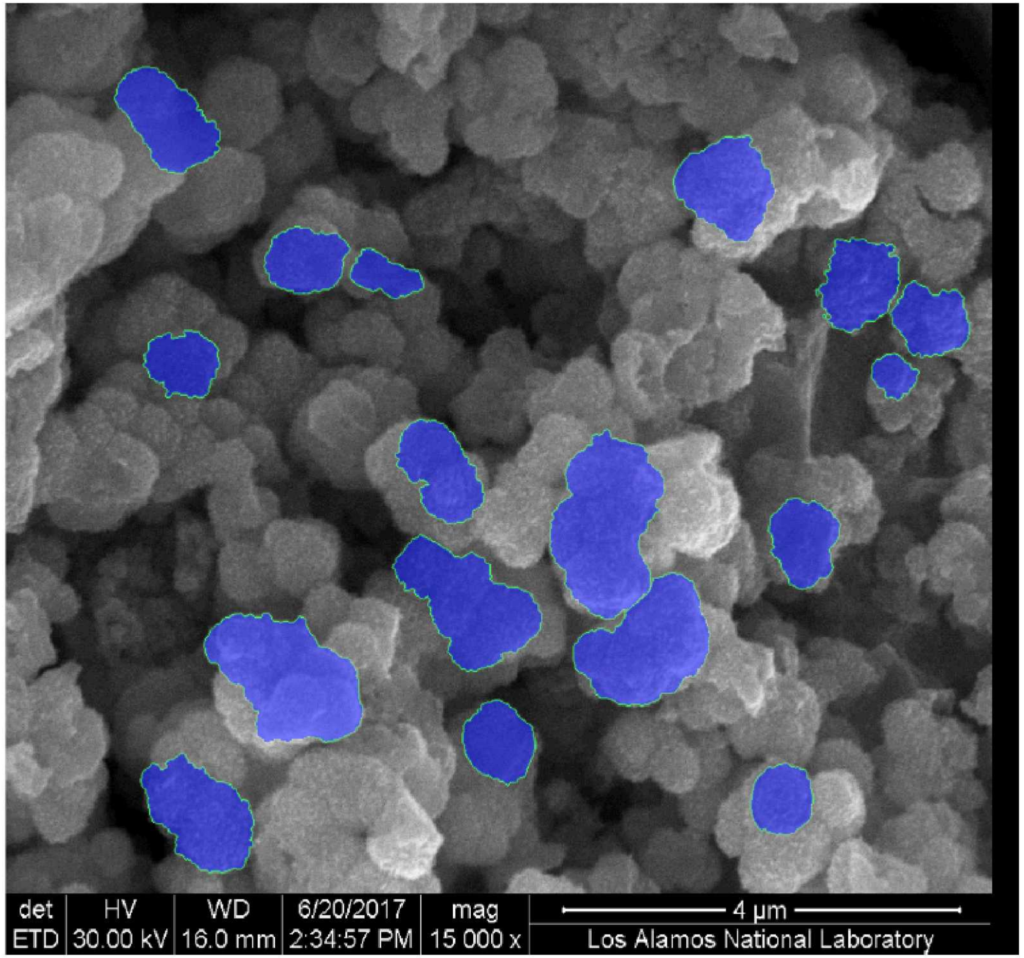
- **Standard method uses means of the distributions as the responses**.
- Standard-5 Y: Responses used are vector area, ellipse aspect ratio, perimeter convexity, ecd, area convexity
- Functional-5 Y: Functional method using vector area, ellipse aspect ratio, perimeter convexity, ecd, area convexity
- Functional-3 Y: Functional method using only vector area, ellipse aspect ratio, and perimeter convexity
- Functional-1 Y: Functional method using only vector area

Review

1. Down-selecting a useful set of responses
   - Don't know how much material will be available for analysis, need to prioritize
   - Find an informative/discriminating set of responses
2. How good are our predictions?
   - Are there missing responses? Is calibration data useful for interdicted material?
   - Pragmatic approach: Make predictions using several methods, assess consistency across methods.
   - Additionally – consult with subject matter experts
3. Utilizing distributional and functional measurements
   - Utilize all available data
   - Inverse prediction using functional regression

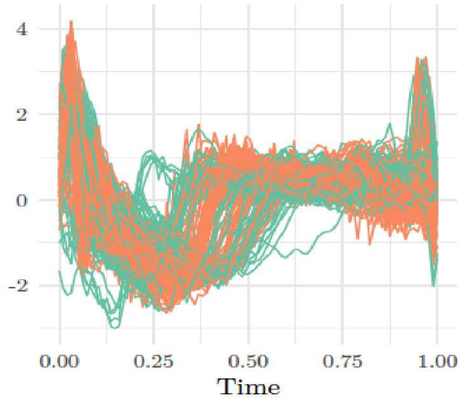
Future Nuclear Forensics Work

- Uncertainty in functional responses
- Shape Analysis
- Image analysis
  - Build on work of Luther McDonald, Tolga Tasdizen at University of Utah
  - Success distinguishing between different production processes using Convolutional Neural Networks
  - Inclusion of other (non-image) responses?

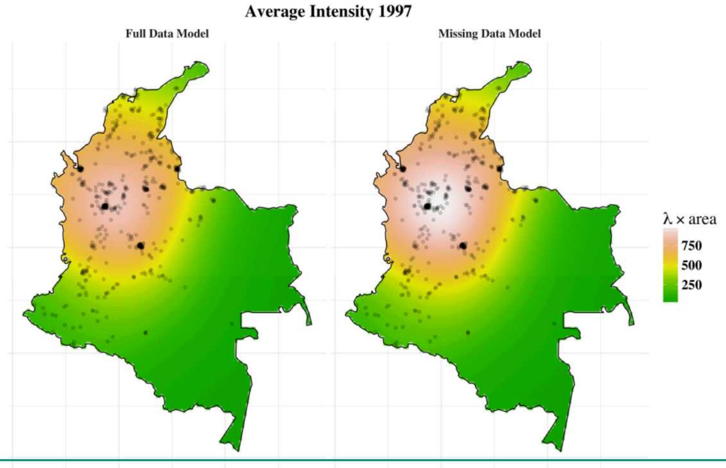


Other Applications

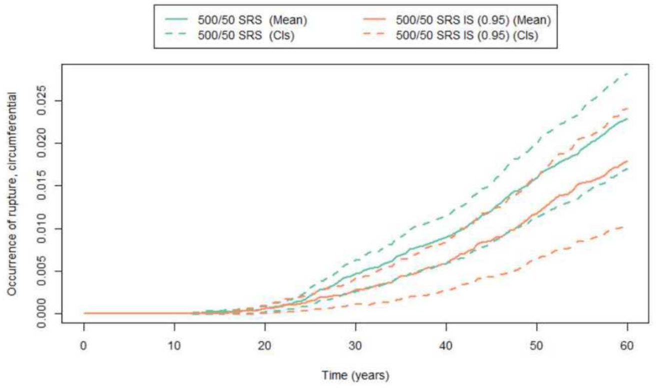
- **Functional data analysis:** Misaligned functional covariates, tolerance bounds



- **Self-exciting point processes** with missing data.



- **Probabilistic Fracture Mechanics**: guidance for power plant safety assessments using PFM models



- **Cyber Analytics** – 250,000,000 attacks on Sandia networks **per day.**
- **Uncertainty Quantification** – Large-scale computer models.
- **Reliability Analysis** – assessing performance of highly-reliable systems

References/Collaborators

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Other Applications

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- J. D. Tucker, Lyndsay Shand, and John R. Lewis. Bayesian modeling of self-exciting point processes with missing temporal histories. (*Submitted*)
- John R. Lewis, Dusty Brooks, and Michael L. Benson. Methods for uncertainty quantification and comparison of weld residual stress measurements and predictions. ASME 2017 Pressure Vessels and Piping Conference, 6B: Materials and Fabrication, 2017.
- Aubrey C. Eckert-Gallup, John R. Lewis, Nevin S. Martin, Lauren B. Hund, Andrew J Clark, Dusty M. Brooks, and Paul E. Mariner. xLPR scenario analysis report. SAND2017-2854, Sandia National Laboratories, Albuquerque, New Mexico 87185 and Livermore, California 94550, March 2017.

Additional slides

Estimating V

To estimate V, first decompose d_i:

$$d_i = \lambda_i + \omega_i - \epsilon_i^* \text{ where,}$$

$$\lambda_i = f_i(\hat{\beta}_i, \hat{X}) - f_i(\beta_i, \hat{X}) \quad \text{and} \quad \omega_i = f_i(\beta_i, \hat{X}) - f_i(\beta_i, X^*)$$

Interpretation of components of d_i

- $\lambda_i = f_i(\hat{\beta}_i, \hat{X}) - f_i(\beta_i, \hat{X})$: error due to uncertainty in model parameters
- $\omega_i = f_i(\beta_i, \hat{X}) - f_i(\beta_i, X^*)$: error due to uncertainty in the candidate solution $\hat{X}$

Assuming properly specified models and unbiased solutions: $E(d_i) = 0$ and

$$V = V_\lambda(\hat{X}) + V_\omega(\hat{X}) + 2cov_{\lambda\omega}(\hat{X}) + V_\epsilon$$

V_λ, V_ω can be estimated using first order approximations, can use residuals to estimate V_ϵ

Simplifying assumptions: $V_\lambda, V_\omega, V_\epsilon$ assumed diagonal, covariance 0.

Solution considers the uncertainty in predicted response – switch role of X and β, related to "errors-in-variables" literature

Forward Models – Linear Main Effects Models

$$\hat{Y}_i = \hat{\beta}_{i0} + \hat{\beta}_{i1}X_1 + \hat{\beta}_{i2}X_2 + \hat{\beta}_{i3}X_3$$

Property: $i = 1, \ldots, 6$	$\hat{\beta}_0$	$\hat{\beta}_1\ (Na_2O)$	$\hat{\beta}_2\ (Ba0)$	$\hat{\beta}_3\ (Al_2O_3)$	$\hat{\sigma}_\varepsilon$	R^2
1. Coeff. of Thermal Exp. (α)	155.8 (6.1)	70.59(10.3)	----	-216.5(31)	3.12	0.86
2. Softening Temp. (T_s)	392.7(15.5)	-104.7(24.6)	----	694.6(63)	5.73	0.93
3. Glass Transition Temp. (T_g)	374.8(14.7)	-104.5(23.7)	----	412.1(66)	6.39	0.82
4. Crystallization Temp. (T_x)	570.5(28.9)	-219.5(48.5)	----	709.8(147)	14.7	0.74
5. Density (ρ)	2.534(0.022)	----	1.113(0.051)	0.484(0.119)	0.0119	0.97
6. Index of Refraction (n)	1.498(0.003)	0.0097(0.004)	0.0834(0.005)	0.1036(0.0123)	0.00113	0.97

For Main Effects Forward Models: $\hat{J}_{ij}(\hat{x}^*) = \hat{\beta}_{ij}$

For this example: $\hat{V} = \hat{V}_\epsilon = \text{diag}(\hat{\sigma}_i^2, i = 1, 2, \ldots, 6)$

$$\hat{C}_{\hat{x}^*} = \left(\hat{J}^T(\hat{x}^*)\hat{V}^{-1}\hat{J}(\hat{x}^*)\right)^{-1} = \left(\hat{B}^\top \hat{V}^{-1}\hat{B}\right)^{-1}$$