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Reverse engineering material processing conditions through inverse prediction using particle shape analysis

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SIAM IS 22 - Virtual

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Outline

Motivation

Elastic Shape Analysis

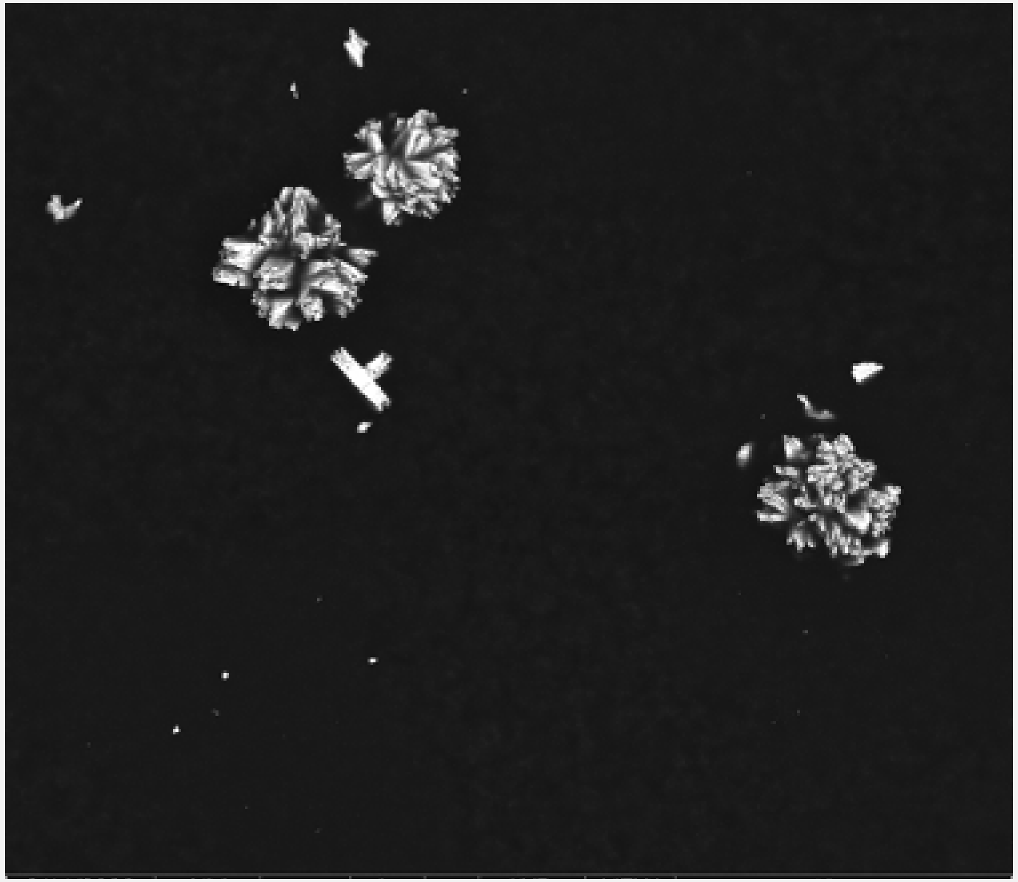
Inverse Prediction Model

Results

Conclusion

Motivation

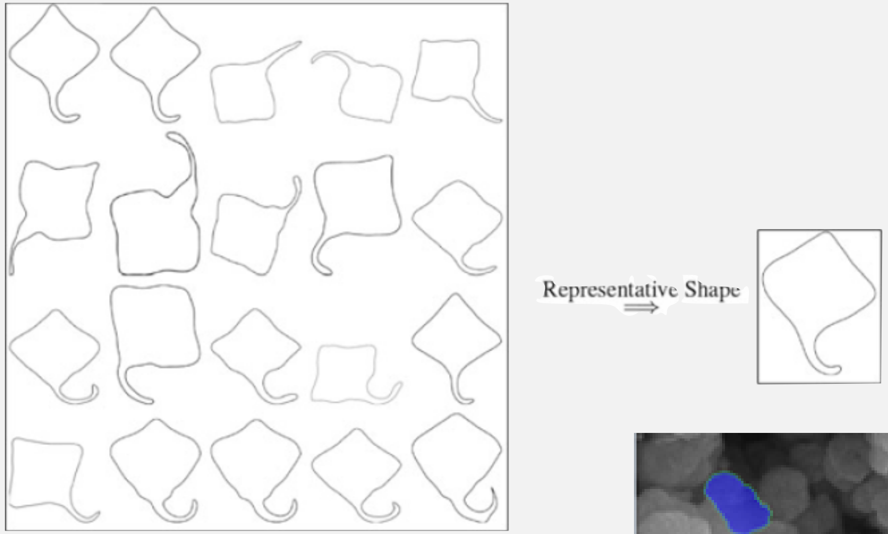
Can we represent crystalline structure via shape information to help us infer processing conditions?



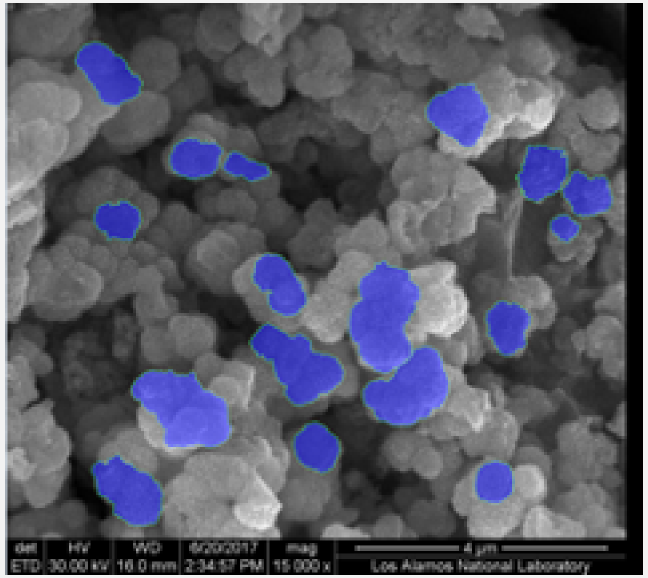
Introduction

- Knowledge about processing conditions helpful in determining material ordination
- This can be considered an **Inverse Problem**
- Our approach is to utilize the ***shape*** of a particle as a predictor in processing conditions
  - Previous work has focused on “features” of shape, but not a mathematical representation of shape itself
  - Utilize Elastic Shape Analysis framework

Shape Analysis



Samples from a population of stingrays from the Surrey fish database on the left and a representative shape for this sample on the right (Srivastava & Klassen 2016)



- Shape analysis of curves is important in various areas such as computer vision, medical diagnostics, and bioinformatics
  - Basic idea is to obtain a boundary curve of an object in a 2D image and analyze those curves to characterize the original object
- Due to functional nature, they live on a non-linear infinite-dimensional space known as a manifold
- We can endow this space with a metric that allows us to measure distances between curves
  - Riemannian framework
- Use metric that is **invariant to rotation, scale, and parameterization of the shape**

Shape Metric and Geodesic

Represent each contour, $\beta(t)$, using the square-root velocity function

$$q(t) = \frac{\dot{\beta}(t)}{\sqrt{|\dot{\beta}(t)|}} = \sqrt{r(t)}\Theta(t)$$

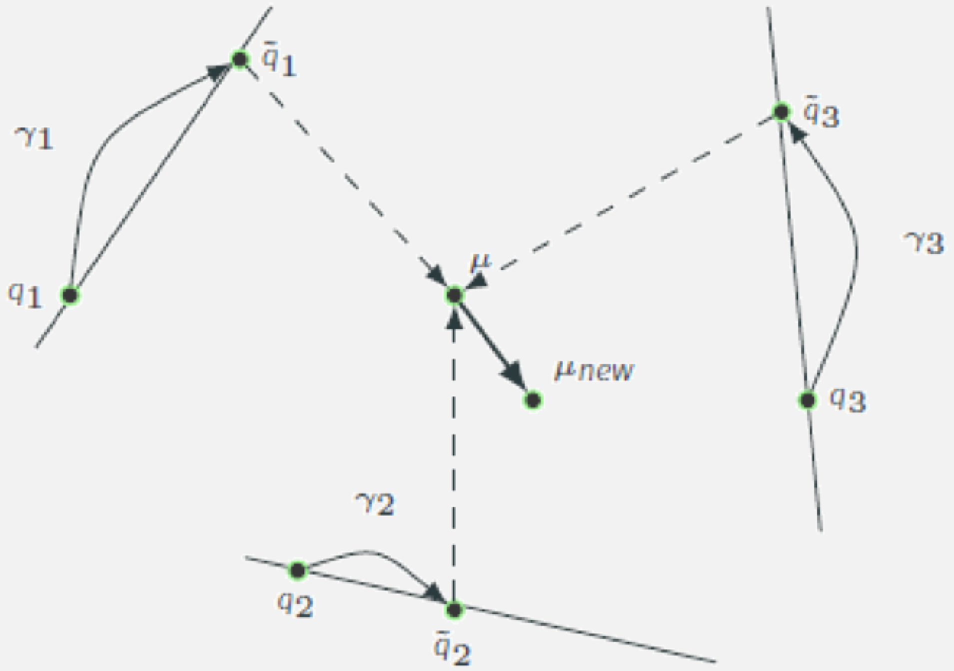
Define the pre-shape space of all unit length contours

$$\mathscr{C}^c = \{q \in \mathbb{L}^2([0,1], \mathbb{R}^n) \,|\, \int_0^1 ||q(t)||^2\, dt = 1, \int_0^1 q(t)||q(t)||\, dt = 0\}$$

Where we define an orbit == a **shape**

$$[q] = \{O(q \circ \gamma)\sqrt{\dot{\gamma}} \,|\, O \in SO(n), \gamma \in \Gamma\}$$

Karcher Mean



From this we can compute a distance between shapes:

$$d_s([q_1],[q_2]) = \min_{O \in SO(n),\, \gamma \in \Gamma} d_c(q_1, O(q_2 \circ \gamma)\sqrt{\dot{\gamma}})$$

Can compute an average curve by computing the **Karcher Mean**, μ

$$\mu = \arg\min_{[q] \in S^c} \sum_{i=1}^{n} d_s([q],[q_i])^2$$

This mean represents the average **shape** of all the curves in the data set

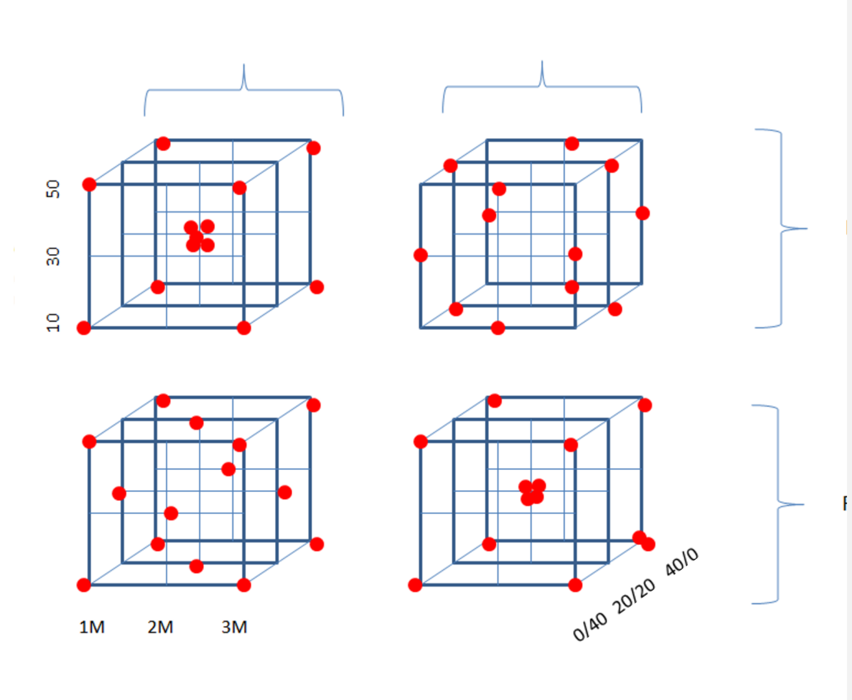
Designed Experiment

I-optimality: minimized average prediction uncertainty.

Sample sizes were chosen to make prediction performance balanced across design space.

Well-designed experiments help to:

- Characterize the input/output relationship
- Increase precision of inverse predictions



Inputs

In solution (52 runs)

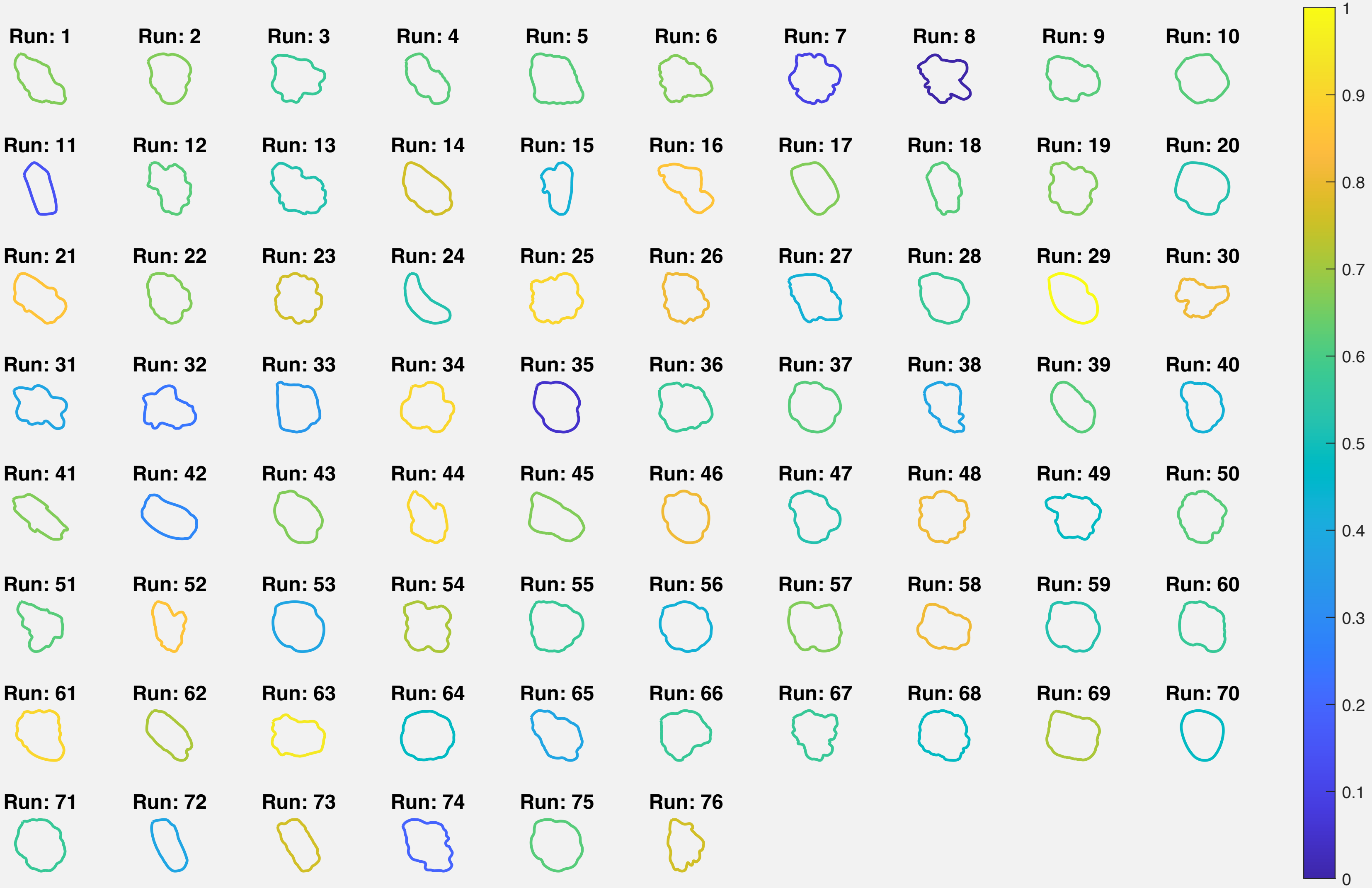
- Parameter 1: 10/30/50
- Parameter 2: 1/2/3
- Parameter 3: direct/reverse
- Parameter 4: 0/20/40
- Parameter 5: 40/20/0
- Parameter 6: 30/50

In solid feed (24 runs)

- Parameter 1: 10/30/50
- Parameter 2: 1/2/3
- Parameter 3 30/50

All particles observed within a run were produced from the same set of processing conditions.

Karcher Means



Colored by relative variability

- The number of PCs to represent 95% of the variation.
- Relative to Run 29 which required the most and Run 8 which required the least

Prediction Results

- Using observed values with missing values imputed from plan and standardized inputs
- Removed condition 5 due to high correlation to condition 6
- Left duplicated runs out, fit model on rest of the runs and predicted the left out run and computed the prediction error
- Performed LOOCV on a **Random Forest Regression** and below is the average standardized RMSE

Solution

	Condition 1	Condition 2	Condition 3	Condition 4	Condition 5
RMSE	0.089	0.097	1.018	0.024	0.099

Solid

	Condition 1	Condition 2	Condition 3
RMSE	0.057	0.188	0.617

Conclusions and Future Work

- Utilized entire curve extracted from SEM imagery in prediction of processing parameters using elastic framework
- Data was extracted using an I-optimal design of experiments
- Results show promise in prediction of parameters using Random Forest Regression model
- Can be combined with other measures for increased performance

Question?

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