Gaussian Process Dynamical Models for designing multi-stage manufacturing process

M.S. thesis defense

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Background

Real-world phenomena

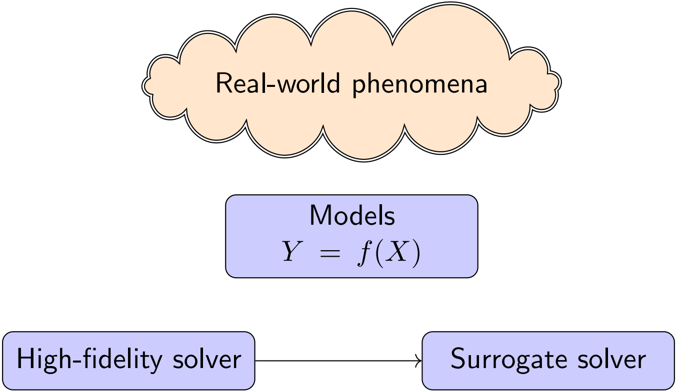
Models

$$Y = f(X)$$

High-fidelity solver → Surrogate solver

- Computational cost
- Inverse problems

Background



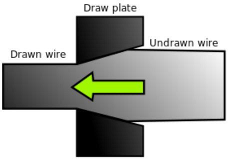
- Computational cost
- Inverse problems

Overview

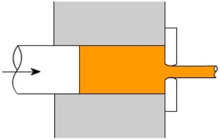
1. Theme
2. Research question
3. Wire drawing
4. Wire drawing results
5. Extending to multi-stage manufacturing

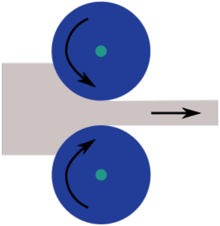
Multi-stage manufacturing

- Definition: Substrate transformation via sequence of similar processes (Mathematical model)



Multi-stage manufacturing processes





Multi-stage manufacturing

Multi-stage manufacturing process

Finite element models
$Y = f(X)$

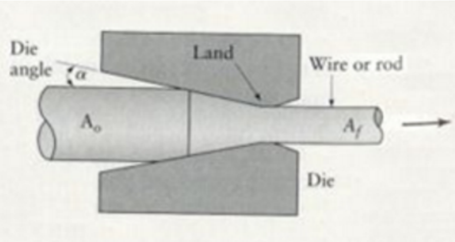
Surrogate solvers:
Response surface
Neural networks
Kriging

Research questions

- How to quantify effect of manufacturing setup design variables on product quality in multi-stage manufacturing processes?
- How to optimize apparatus design parameters for attaining desired substrate properties?

Wire drawing

- Successive die passes for wire diameter reduction
- Finite element simulation
  - FE mesh
    (1) Topology: Node and connectivity
    (2) Field: Stress/Strain/Temperature data
  - Material properties at each pass
- Goal: Build surrogate model for FE solver to predict material properties



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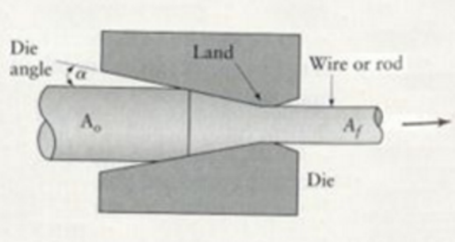

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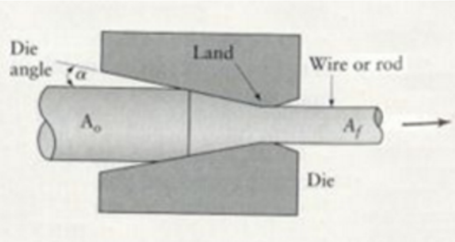
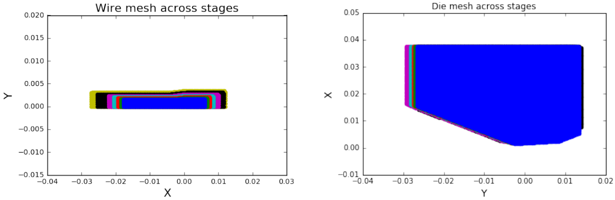


Wire drawing

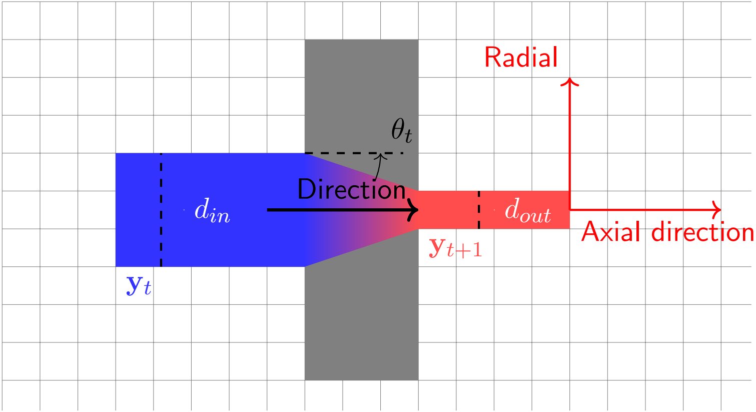
- Wire and die mesh at each pass
- Finite element simulation
  - Extrusion mesh
    1. (1) Topology: Node and connectivity
    2. (2) Field: Stress/Strain/Temperature data
  - Material properties at each pass



(a) Multiple wire meshes. (b) Multiple die meshes.

Dynamic modeling

- Inputs at stage t ($\mathbf{u}_t$) : θ_t, $r_t = (\frac{d_{in}}{d_{out}})^2$



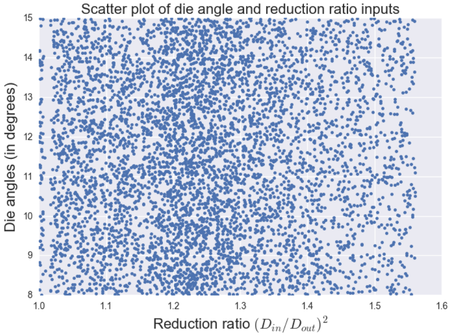
Design of experiments

Experiments with Finite element solver as true value

- Output variables : Stress/Strain/Temperature at FE nodes in each pass
- Input factors:

Number of stages	$\{4, ..., 8\}$
Input wire diameter (in mm)	$[4, 24]$
Die angle (in degrees)	$[8, 15]$
Reduction ratio $((D_{in}/D_{out})^2)$	[1.04, 1.56]

Scatter plot of die angles and reduction ratio to evaluate FE solver



Modeling approach for wire drawing

(1) Spatial representation

(2) Dimensionality reduction

- Spatial symmetry
- Constitutive laws

Using principal component analysis

- Existence of linear manifold

(3) Regression map in low-dimensional space

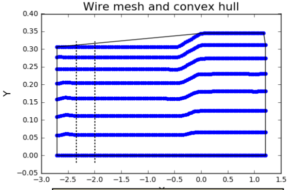
Using Gaussian processes for reduced space dynamical map

- Quantifying epistemic uncertainty
- Enabling stochastic optimization

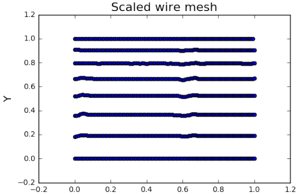
(4) Reconstruction

Spatial representation of wire mesh

- Wire mesh representation with finite element nodes
  - Transformation: Normalization from mesh boundary
  - Selection: Choose smallest subset of nodes representing substrate



Original FE mesh



Transformed wire space

- Transformation equation

$$\mathbf{D}_{ij} = \{\mathbf{X}_{ij}, \mathbf{Y}_{ij}\}$$

Spatial representation of wire mesh

- Representing wire “state”: Collating relevant nodal properties
- Input dimensionality: 288 (16 nodes, 18 nodal properties)

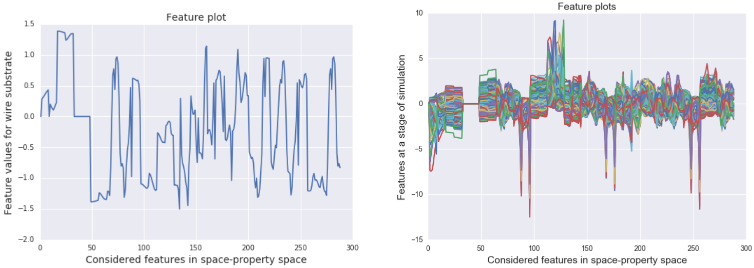


Figure: Scaled feature values for wire at stage of manufacturing

Notation for dynamical formulation

- t: Stage (Pass) number $\{0, 1, 2, \cdots\}$
- u_t: Design variables at stage t [Die angles(θ_t), Reduction ratio (r_t)]
- y_t: Wire "state" at stage t [Stress, strain, displacement, temperature]
- x_t: Wire "state" in reduced dimensions at stage t (PCA descriptors)
- z_t: Relevant properties at stage t (Ex- Ultimate tensile strength)

Dynamics:

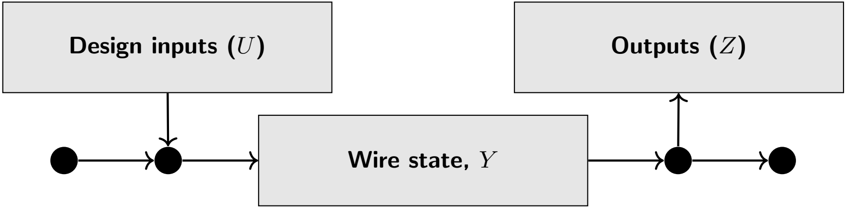
$$\mathbf{y}_{t+1} = \tilde{f}(\mathbf{y}_t, \mathbf{u}_t)$$

Dynamics:

$$\mathbf{y}_{t+1} = \tilde{f}(\mathbf{y}_t, \mathbf{u}_t)$$

(+) Input diameter
(+) Die angles
(+) Reduction ratio
(+) Draw speed

(+) Energy
(+) Draw force
(+) Maximum temperature
(+) Ultimate tensile strength



(+) Geometry(Coordinates)
(+) Properties (Stress, Displacements)

Equations

Dynamics:

$$\mathbf{y}_{t+1} = \tilde{f}(\mathbf{y}_t, \mathbf{u}_t)$$

Dimensionality reduction map:

$$\mathbf{x}_t = \mathbf{g}(\mathbf{y}_t)$$

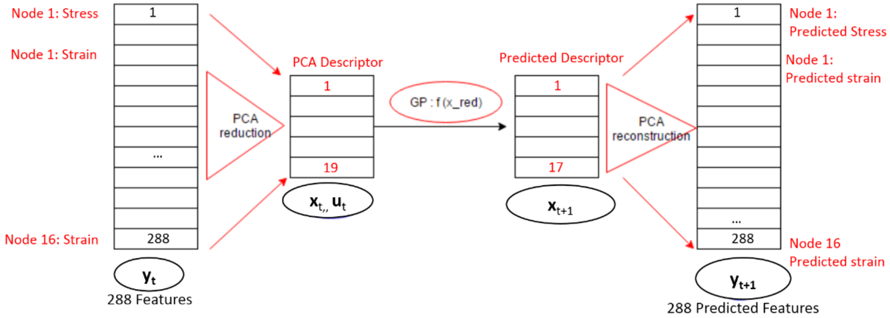
State equation:

$$\mathbf{x}_{t+1} = f(\mathbf{x}_t, \mathbf{u}_t)$$

Property equation:

$$\mathbf{z}_t = \mathbf{h}(\mathbf{x}_t)$$

Dynamics in reduced space



Dimensionality reduction: Principal component analysis

Accuracy of reduction reconstruction map

$$\mathcal{C}(\mathcal{R}(\mathbf{y}_k)) \approx \mathbf{y}_k$$

Projecting vector $\mathbf{y}_k$ along principal components:

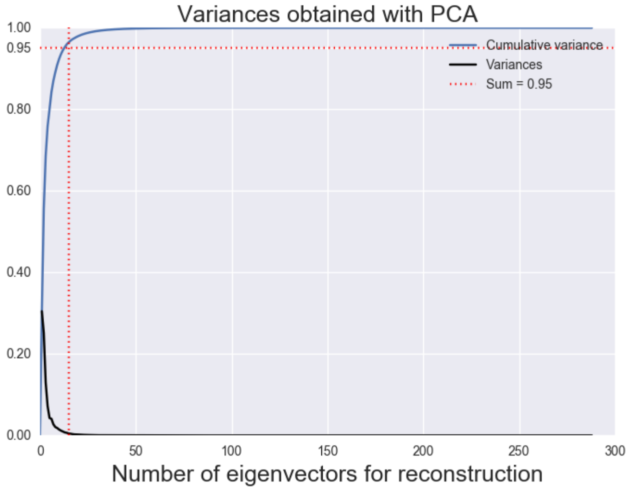
$$\mathbf{x}_k = \mathbf{W}_R \cdot \mathbf{y}_k$$

$$\tilde{\mathbf{y}}_k = \mathbf{W}_C \cdot \mathbf{x}_k$$

Select columns of $\mathbf{x}_k$ based on variance along each component

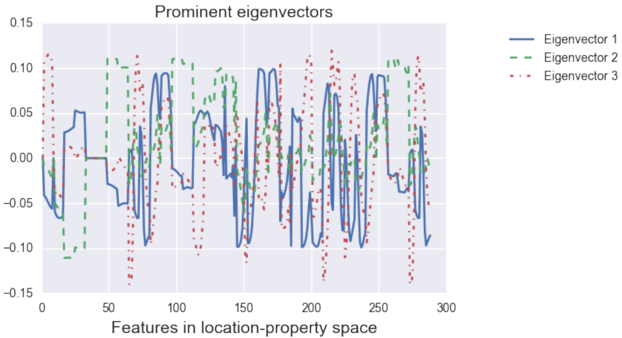
PCA on wire drawing

- Correlation matrix across features in training data set
- Score plot: Selecting 17/288 descriptors



PCA on wire drawing

Sample eigenvectors as components



Validating PCA in wire drawing

- Comparing originals (green) with reduced-reconstructed feature (blue)
- Score value = 0.97

Gaussian process regression

- Learn regression map between scaled inputs and outputs across dies in low-dimensions

$$\mathbf{x}_{t+1} = \mathbf{f}(\mathbf{x}_t, \theta_t, r_t)$$

- Assume zero-mean Gaussian process with Squared-exponential kernels for each output dimension r,

$$f_r \sim GP(f_r|0, c(\cdot, \cdot; \phi_r)) \quad \text{where}, r = \{1, \cdots, d_y\}$$

- Learn optimal hyperparameters (ϕ_r) and add observations to trained Gaussian process

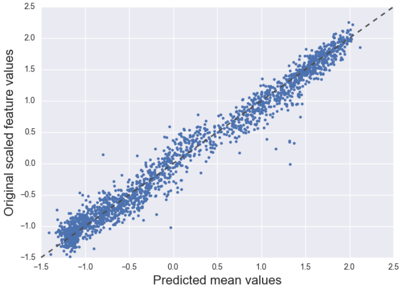
Validating GPR results

Expensive steps in Gaussian processes

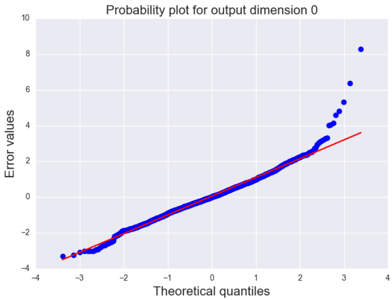
- Inverse of covariance matrix: Only for training observations
- Optimizing hyper-parameters: Can be used for adding observations

Validation in first output dimension

- Scatter plot for predicted and original samples



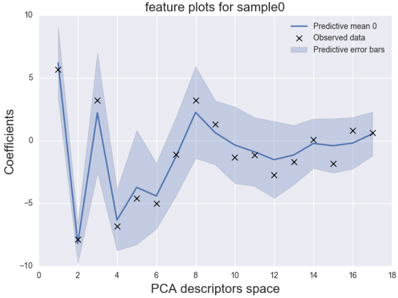
- Quantile plots for predicted and original samples



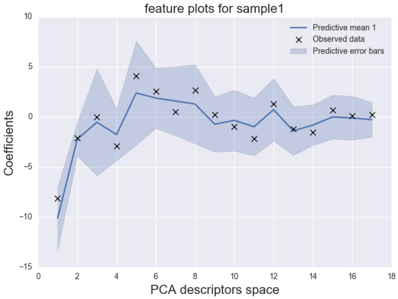
GPR prediction samples

Comparing predictions from GP maps in low-dimensional space

- Sample 1 for GP regression map



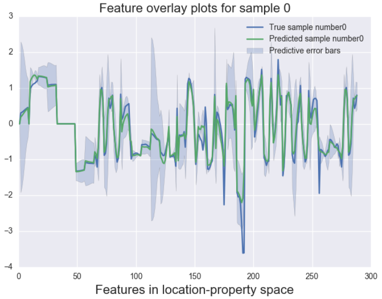
- Sample 2 for GP regression map



Step predictions

- Predicting step-ahead properties for validation
- Steps: PCA reduction → GP regression → PCA reconstruction
- Prediction quality correlated with input sequence and stages

- Sample 1 for step ahead predictions



- Sample 3 for step ahead predictions

Prediction on wire properties

Single step ahead wire property prediction

$$\tilde{\mathbf{z}}_{k+1} = \mathbf{h}(\mathbf{f}(\mathcal{R}(\mathbf{y}_k), \mathbf{u}_k))$$

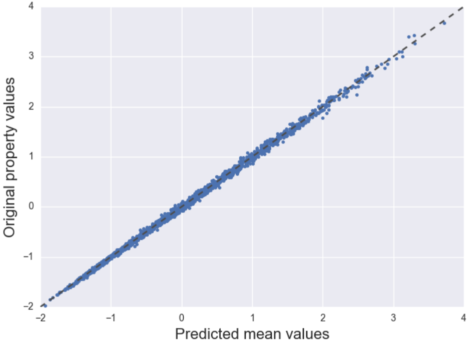


Figure: Validating single stage predictions of Ultimate tensile strength on verification data set.

Multi-stage predictions, uncertainty quantification and propagation

- Plotting prediction uncertainties after multiple stages
- Comparisons across features and stages of prediction
- 18 properties: Stress, strain, temperature

- Monte-carlo simulations for generating sample paths for initial wire features $\mathbf{y}_0$ and inputs $(\mathbf{u}_0, \mathbf{u}_1, \cdots)$

$$\tilde{\mathbf{y}}_{k+1} = \mathcal{C}(\mathbf{f}(\mathcal{R}(\mathbf{y}_k), \mathbf{u}_k))$$

Results

(1) Effects of training dataset size on prediction error

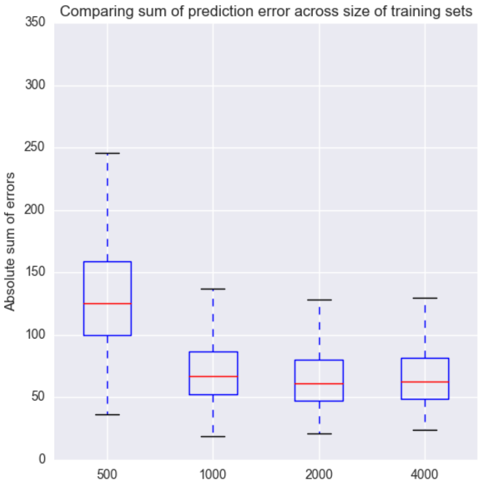
(2) Feature space predictions for a drawing setup

(3) Feature specific uncertainty propagation

(4) Wire property optimization

1. Uncertainty quantification and training size

Comparisons over a prediction data set



2. Feature space predictions for a drawing setup

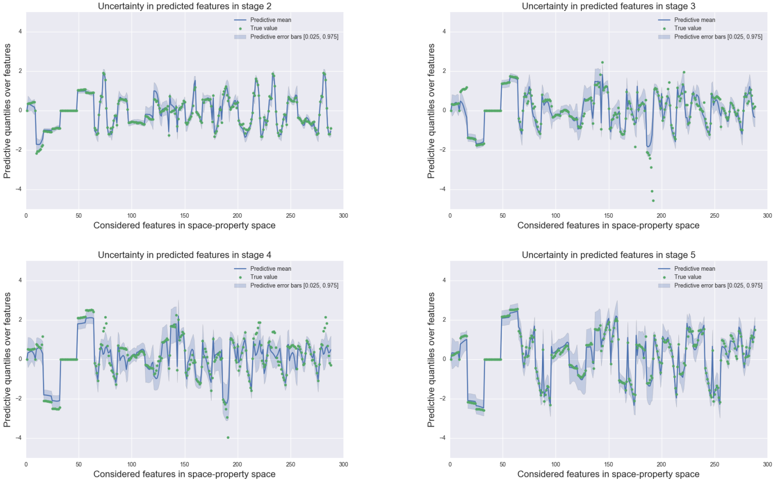
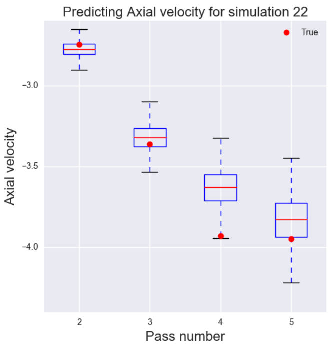
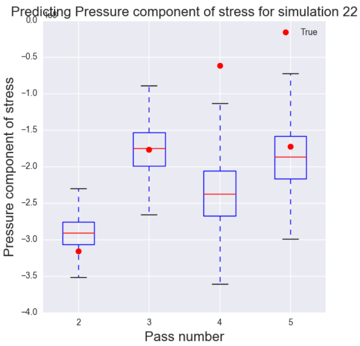


Figure: Multi stage predictions for wire drawing setup 22.

3. Feature specific uncertainty propagation

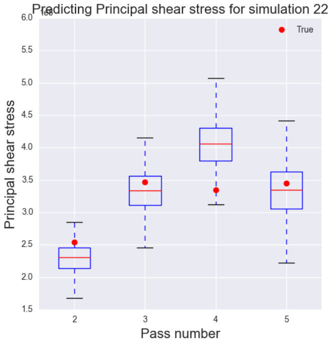


(a) Axial velocity.

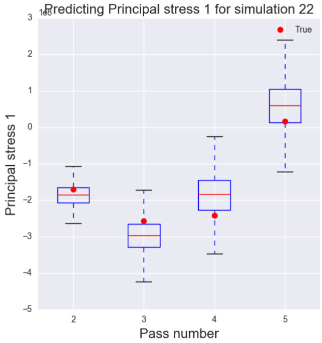


(b) Pressure component of stress.

3. Feature specific uncertainty propagation



(c) Principal shear stress.



(d) Principal stress.

4. Optimization

- Optimize "Expected ultimate tensile strength" (z_T) of final product
- Using surrogate model made with GP and PCA
- Design variables: Die angles $(\theta_0, \cdots, \theta_T)$

Where single step-ahead property prediction is given as,

$$\tilde{\mathbf{z}}_{k+1} = \mathbf{h}(\mathbf{f}(\mathcal{R}(\mathbf{y}_k), \mathbf{u}_k))$$

Table: Details of simulation setup 7 in validation data set.

#	Stage 1	Stage 2	Stage 3	Stage 4	Stage 5
Diameter sequence	14.14	13.50	11.90	10.30	10.13
Die angles	-	13.89	13.43	12.55	9.016

4. Optimization

Table: UTS improvement in multi-parameter simulation

#	Die Angle (degrees)	Expected UTS (GP Model)	UTS (FE Model)	Function evaluations
Original	[13.9, 13.43, 12.5, 9.0]	1627.72	1610	-
Basin-hopping	[12.6, 11.9, 11.84, 13.66]	1640.17	1611	1438
Differential Evolution	[12.76, 14.89, 14.92, 14.01]	1663.37	1625	1651
Random search	[14.14, 14.73, 14.97, 14.65]	1657.53	1622	1000

- Differential evolution optimizes better due to exploration based strategy
- Extension to stochastic optimization: Using predictive variances with Expected improvement based Efficient global optimization

4. Optimization

Table: Run time comparison in multi-parameter simulation

		FE solver	GP solver (MC samples)		
		True	1	100	1000
Evaluations	Single-step	29 s	0.002	0.2	2
	Multi-step (4)	89 s	0.01	1	10
Multi-step (4) Optimization	Basin-hopping (1438 evaluations)	35.55 hrs	-	24 min	4 hrs
	Differential evolution (1414 evaluations)	40.81 hrs	-	27.5 min	4.58 hrs

Summary for wire drawing problem

(1) Spatial representation
- Normalization from boundary to common space
- Selecting least set of nodes for representing substrate "state"

(2) Dimensionality reduction
- Spatial symmetry
- Constitutive laws

Using principal component analysis
- Capturing dynamics in linear manifold

(3) Regression map in low-dimensional space
Using Gaussian processes for reduced space dynamical map
- Quantifying epistemic uncertainty
- Enabling stochastic optimization with predictive variance

(4) Optimization
Global optimization of expected substrate property
- Extension to stochastic optimization

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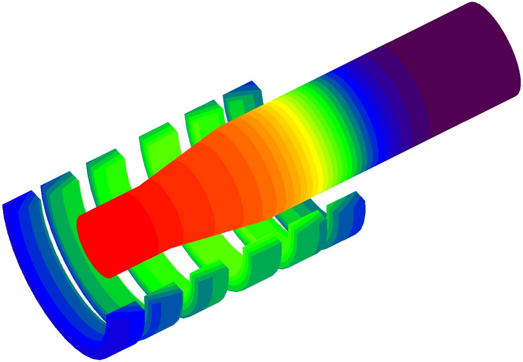
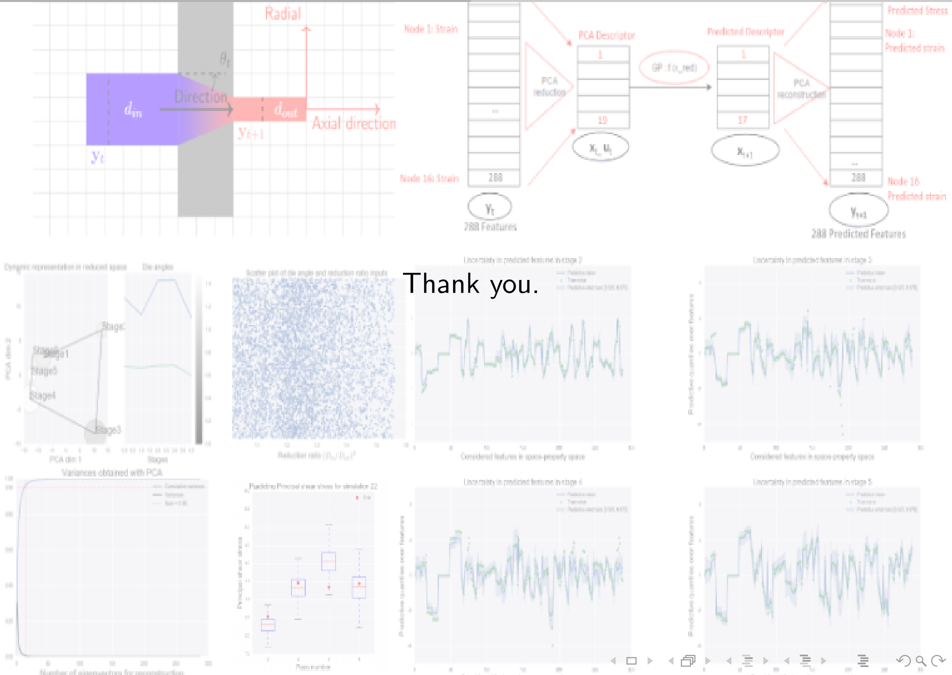
Extending to multi-stage manufacturing processes

Hot rolling



- Spatial representation
- Dimensionality reduction and regression mapping



Thank you.