Department of MECHANICAL ENGINEERING THE UNIVERSITY OF UTAH

Interpretability and Generalizability of Constitutive Models using Symbolic Regression

Jacob Hochhalter, University of Utah

Karl Garbrecht, Donovan Birky, David Randall, Brian Phung, Nolan Strauss, University of Utah

John Emery, Brian Lester, Coleman Alleman, Michael Buche, Sandia National Laboratories

Laurent Capulongo, Andrea Rovinelli, Los Alamos National Laboratory

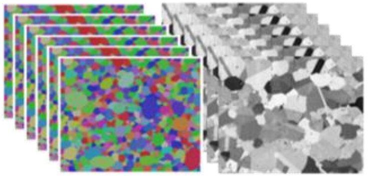
Geoffrey Bomarito, Patrick Leser, NASA Langley Research Center

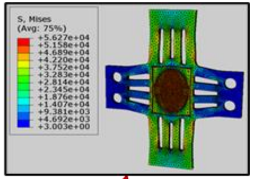
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

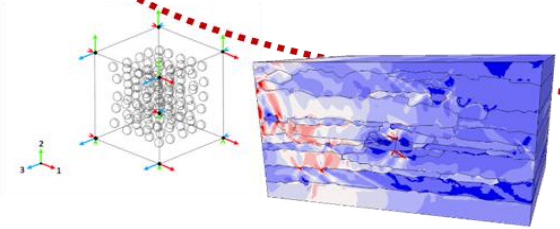
Bingo: https://github.com/nasa/bingo

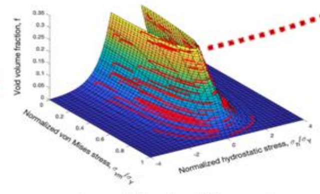
Outline

1. **Interpretable, Data-driven Machine Learning Background**
   - What do we mean by ‘interpretability’ and ‘generalizability’
   - Genetic Programming with Symbolic Regression (GPSR)
   - Data-driven interpretable ML for constitutive models
2. **Laying a Scientific Machine Learning Foundation**
   - Prescribing the model domain with Continuum Thermodynamics
   - Verification studies for ML material models
   - Breaking down microstructure complexity into bite-sized steps
3. **Finite Element Method Auto-implementation**
   - Tensor transform method for surface mapping



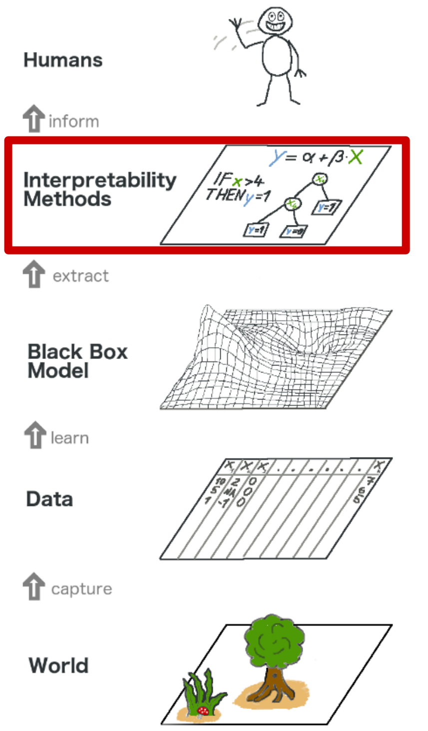






Gurson yield surface in $(\sigma_h, \sigma_{vm}, f)$ space

Machine Learning in Engineering



https://christophm.github.io/interpretable-ml-book/agnostic.html

"Interpretability is the degree to which a human can understand the cause of a decision"[1]

[1]Miller, Tim. (2017) "Explanation in artificial intelligence: Insights from the social sciences." arXiv:1706.07269.

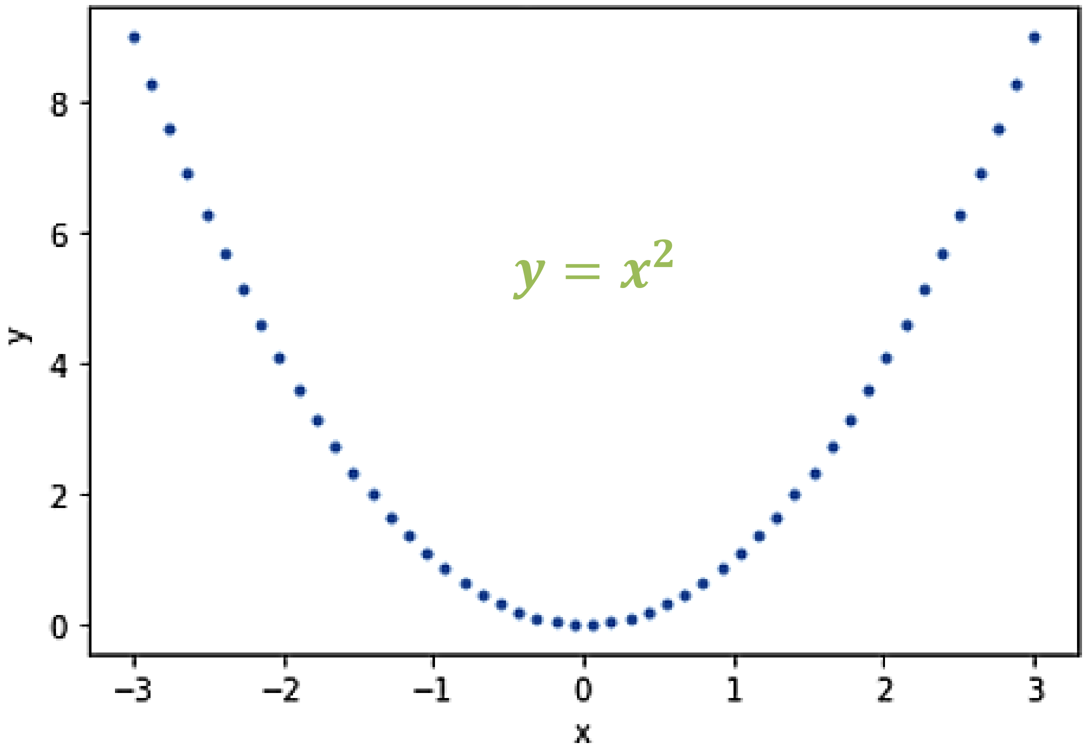
Engineers and scientists seek interpretability for:

- Building trust
- Directing future data collection
- Informing feature engineering
- Informing human decision-making

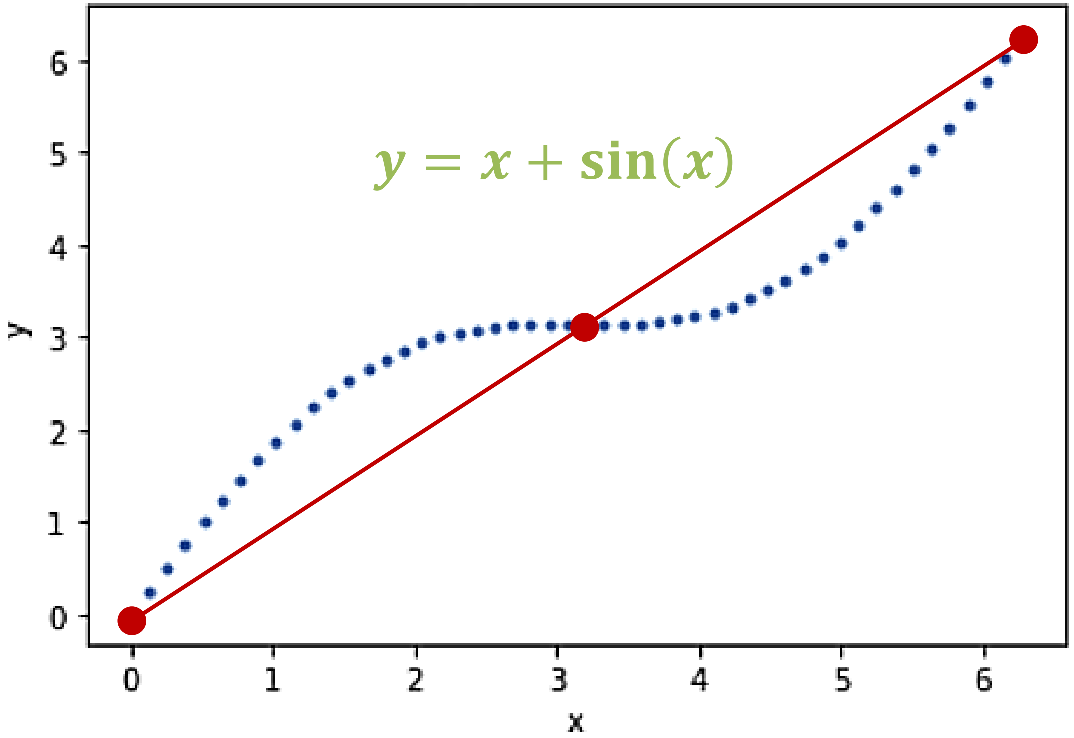
Analytic models are inherently interpretable and common insights, like feature sensitivies, are readily obtained.

Explainable models go beyond the interpretable to enable justification of why a model is generalizable.

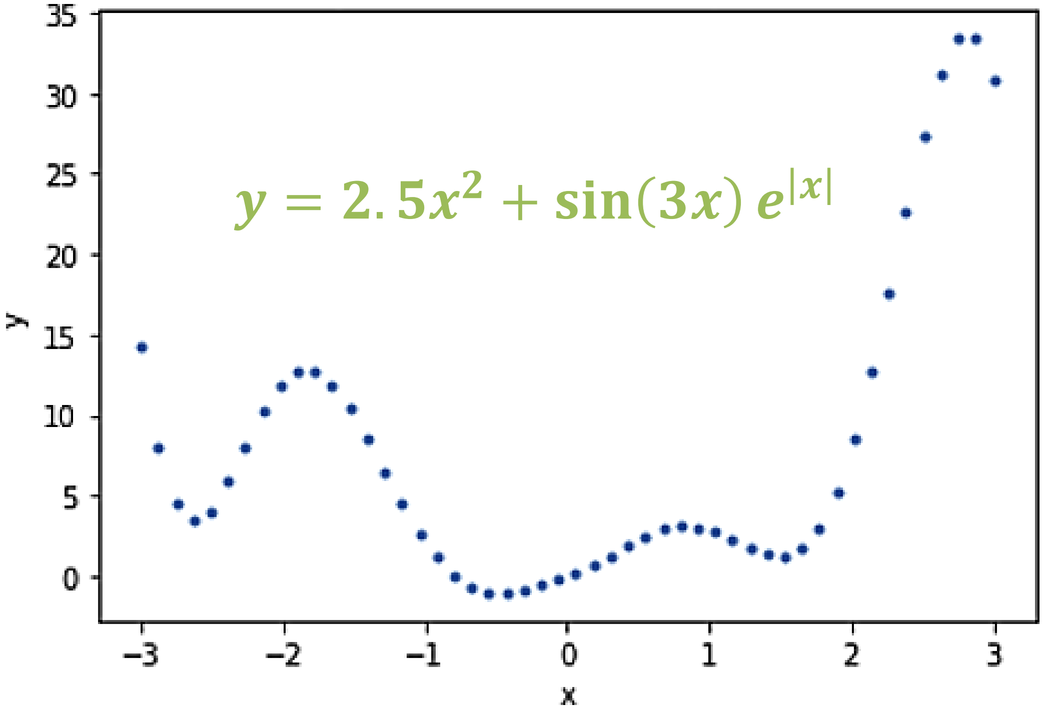
Name That Model



Name That Model

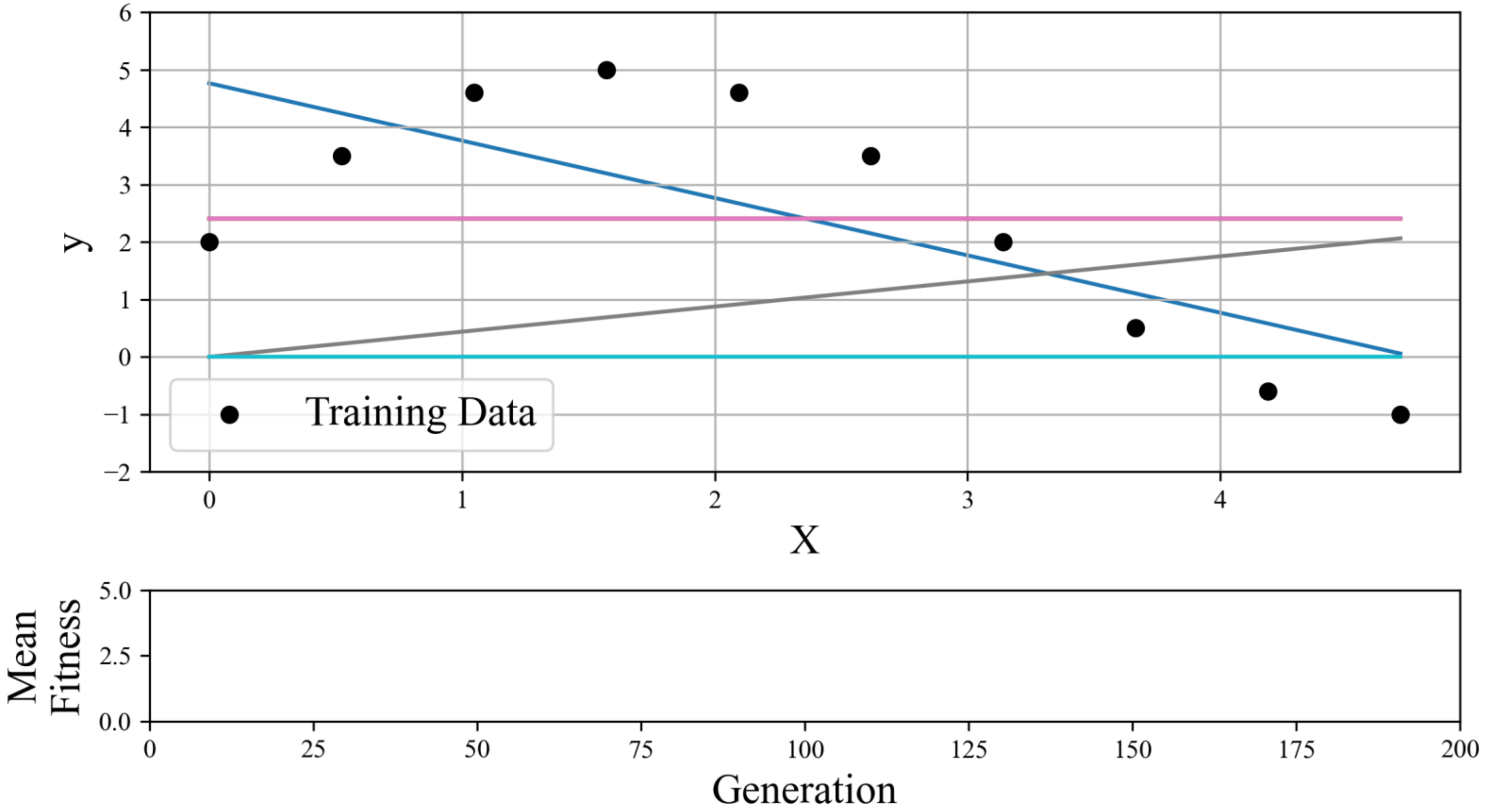


Name That Model



$$y = 2.5x^2 + \sin(3x)\, e^{|x|}$$

Genetic Programming with Symbolic Regression

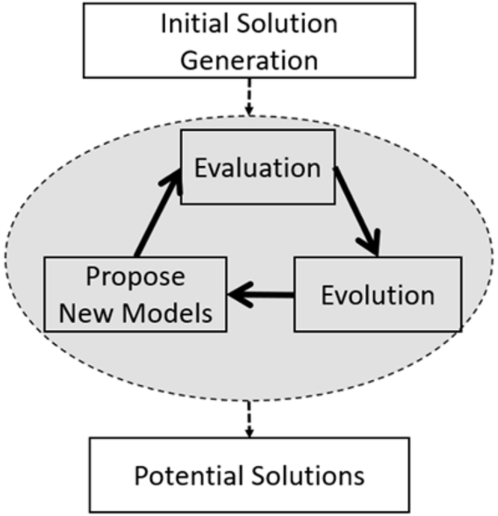


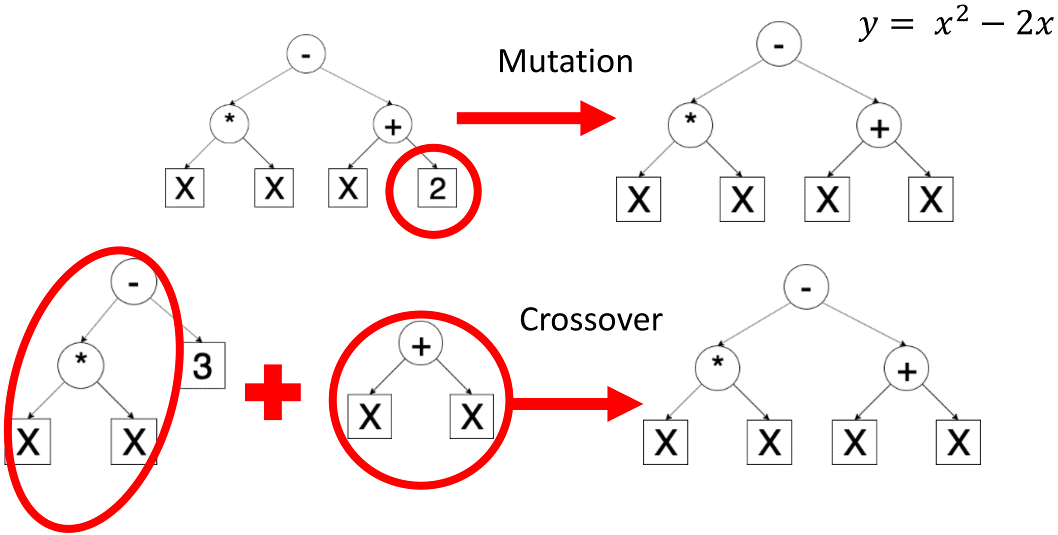
Genetic Programming with Symbolic Regression

GPSR Algorithm Concept

Genetic Programming (GP): Evolution of computer programs
Symbolic Regression (SR): Searching space of mathematical functions
Fitness Function: Definition of how model matches data

(1) generate population of equations, (2) create offspring, (3) evaluate fitness, (4) select equations

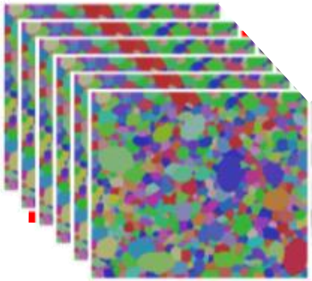




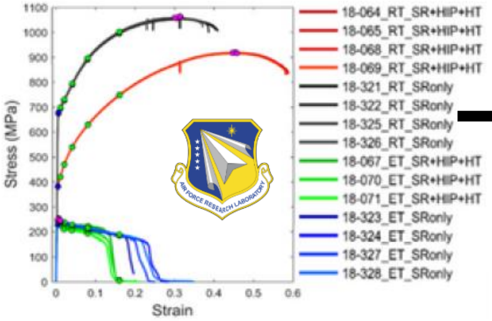
Data-driven GPSR for Hardening

DREAM.3D

EBSD .ctf data ("Middle")

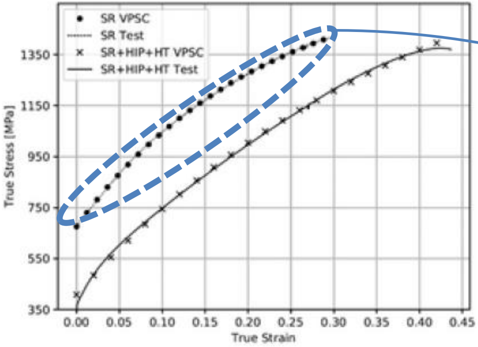


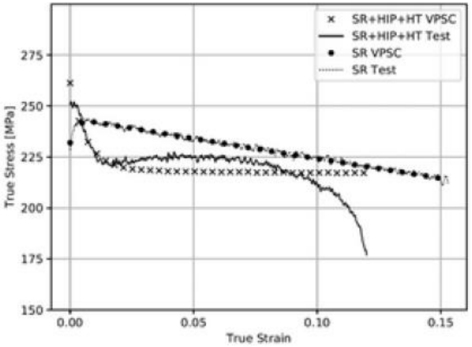
http://dream3d.bluequartz.net/



*VPSC + scipy

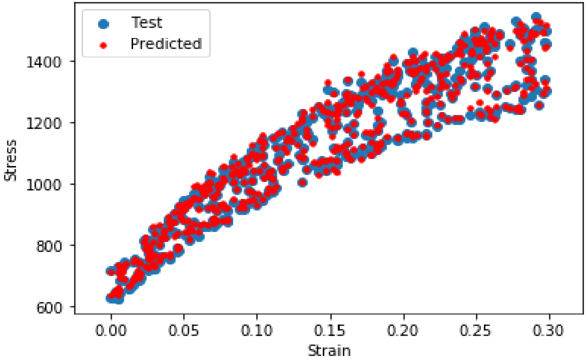
Calibrate VPSC to experiment





Generation 1000 simulated 'Tests'

- Subsample grain orientations
- Test GPSR model against VPSC test simulations



Example for SR at room temperature

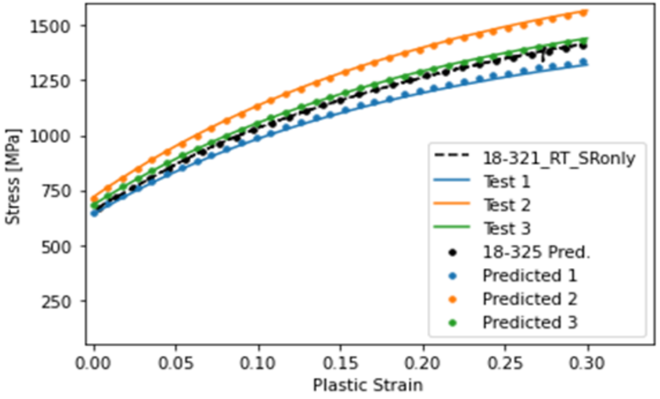
Data-driven GPSR for Hardening

$$\sigma = (-0.16)(-2.5E4 + 1.3E4\alpha) + \left(\frac{\beta}{\cos(\beta)} - \beta\right)(-2.5E4 + 1.3E4\alpha) + (3.6E-3)\left(\sin(-3.7E3 - (\epsilon))\right)(-2.5E4 + 1.3E4\alpha)$$

$$\sigma = c_1 F(\alpha) + G(\beta)F(\alpha) + H(\epsilon)F(\alpha)$$

ε = Plastic Strain (%) **α** = Texture Parameter 1 **β** = Texture Parameter 2

3 Randomly sampled specimen stress-strain testing data vs. GPSR model result



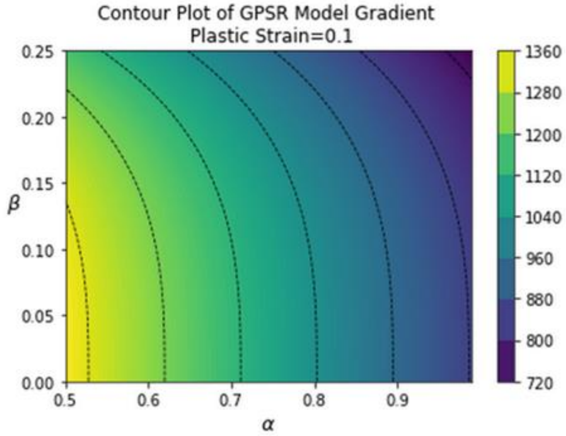
$$\frac{d\sigma_{pred}^{m2}}{d\alpha} = c_1 * 1.26e4 + G(\beta) * 1.26e4 + H(\epsilon) * 1.26e4$$

$$\frac{d\sigma_{pred}^{m2}}{d\beta} = \left(\frac{\beta sin(\beta)}{cos^2(\beta)} + \frac{1}{cos(\beta) - 1}\right) F(\alpha)$$

CV Error Metric	Results
Training MAPE	0.64
Testing MAPE	0.63

MAPE = Mean Absolute Percent Error (%)

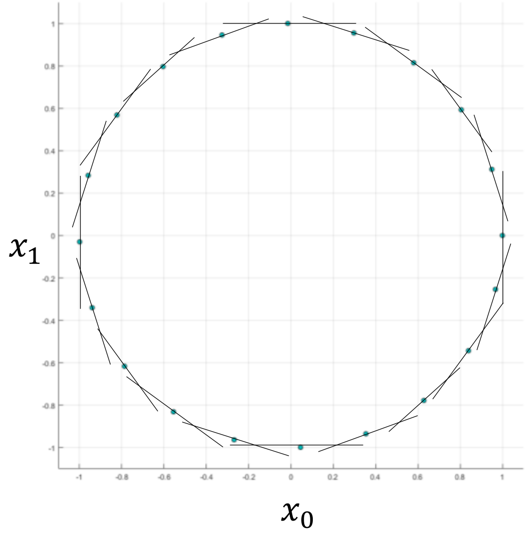
Partial Derivatives w.r.t. texture parameters



Mechanics-driven GPSR for Yield Surface

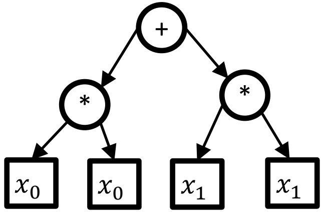
Define fitness for plasticity (implicit) equations

Given data: $X(x_0, x_1)$



Calculate $\frac{\Delta x_0}{\Delta t}$ and $\frac{\Delta x_1}{\Delta t}$

Propose model: $f(x_0, x_1)$



Calculate $\frac{\partial f}{\partial x_0}$ and $\frac{\partial f}{\partial x_1}$

Calculate $\frac{\partial f}{\partial t}$ via chain rule $\frac{\partial f}{\partial x_0}\frac{\Delta x_0}{\Delta t}$ and $\frac{\partial f}{\partial x_1}\frac{\Delta x_1}{\Delta t}$

average normalized deviation of f:

$$E(f, X) = \frac{1}{N}\sum_{i=1}^{N}\left|\sum_{j=1}^{P}\frac{\frac{\partial f}{\partial x_j}\frac{\Delta x_j}{\Delta t}}{\left|\frac{\partial f}{\partial x_j}\frac{\Delta x_j}{\Delta t}\right|}\right|^{(i)}$$

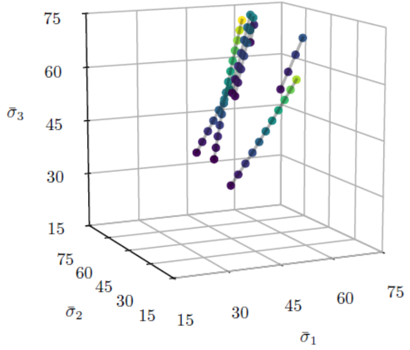
Prager Consistency Condition:

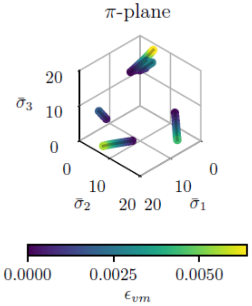
$df = 0$ at yield because $f(\boldsymbol{\sigma}, \boldsymbol{\varepsilon}_p) = 0$

$$df = \frac{\partial f}{\partial \boldsymbol{\sigma}} : d\boldsymbol{\sigma} + \frac{\partial f}{\partial \boldsymbol{\varepsilon}_p} : d\boldsymbol{\varepsilon}_p = 0$$

Verification of IML Constitutive Models

<u>Linear hardening</u>





BINGO →

$$
\begin{aligned}
&\epsilon_{vm} - (\bar{\sigma}_2 - \bar{\sigma}_3 - (\epsilon_{vm} + \bar{\sigma}_2 - \bar{\sigma}_1)) \\
&- ((15.2)((-0.142)(-0.142)) + \epsilon_{vm} + (\epsilon_{vm} + \bar{\sigma}_2 \\
&- \bar{\sigma}_3 - (\epsilon_{vm} + \bar{\sigma}_2 - \bar{\sigma}_1))(\bar{\sigma}_2 - \bar{\sigma}_1) + \epsilon_{vm} - (-33.9) \\
&+ ((\epsilon_{vm} + (-0.142)(-0.142))(\epsilon_{vm} + \epsilon_{vm}))(490100) \\
&+ \epsilon_{vm} + \epsilon_{vm} - (\bar{\sigma}_2 - \bar{\sigma}_3 - (\epsilon_{vm} + \bar{\sigma}_2 - \bar{\sigma}_1) + \epsilon_{vm} \\
&+ (-0.142)(-0.142) + (\bar{\sigma}_2 - \bar{\sigma}_3)(\bar{\sigma}_2 - \bar{\sigma}_3) - \epsilon_{vm})) \\
&= constant
\end{aligned}
$$

<u>Stats</u>:
70 simulated tests
33 points for each test
40 cores
~1 minute for convergence

simplify ↓

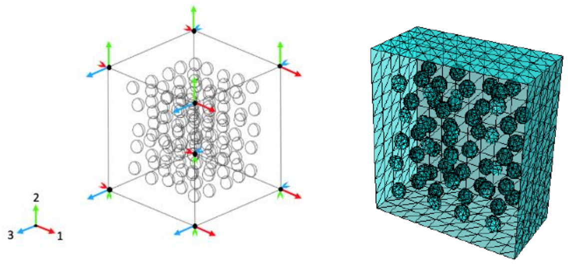
Exact solution form recovered
Coefficients produced result in 0.0001% relative error

$$c_0 + \frac{1}{2}((\bar{\sigma}_1 - \bar{\sigma}_2)^2 + (\bar{\sigma}_2 - \bar{\sigma}_3)^2 + (\bar{\sigma}_3 - \bar{\sigma}_1)^2 \ - c_1\epsilon_{vm} - c_2\epsilon_{vm}^2) = constant$$

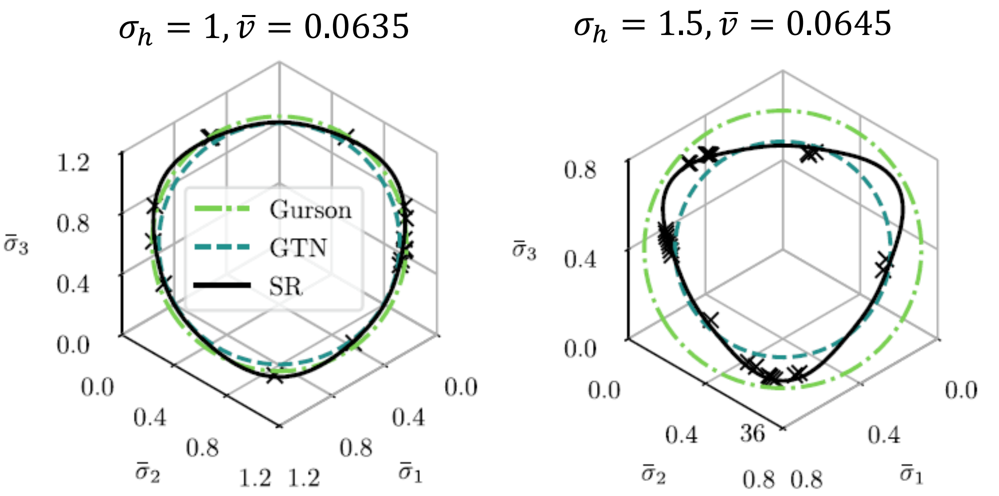
Mechanics-driven GPSR for Yield Surface

Simulated training data:

- Spherical, random void microstructure
- Proportional loading
- Matrix von Mises (perfect) plasticity
- Random perturbations of voids



Stats:
169 simulated tests
145 points for each test
160 cores
~72 hours for convergence



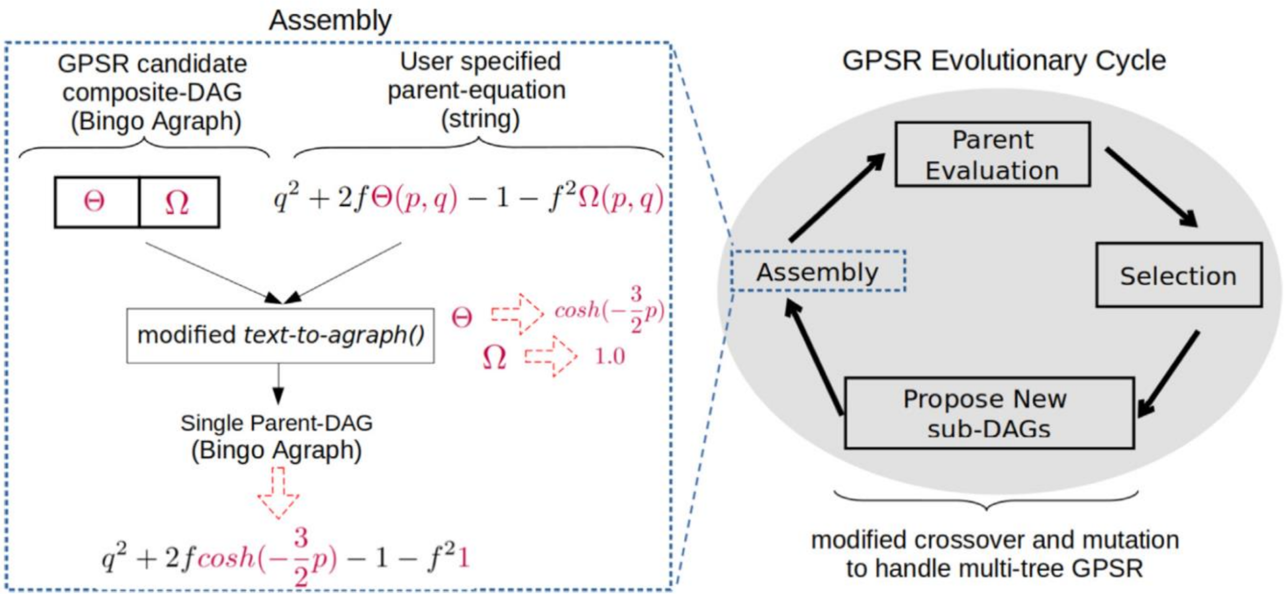
$$\Phi_{SR} = \left[\bar{\sigma}_{vm}(4\bar{\sigma}_h^2 + (2\bar{v} - \bar{L} + c_1)\bar{\sigma}_h + c_2) - \bar{\sigma}_h(c_3\bar{v}^2 + c_4)\right](c_5\bar{v}^2 + 2\bar{v} + c_6) + c_7\bar{v}^2 - \bar{\sigma}_{vm}\bar{L}^2(c_8\bar{v}^2 - c_9) + c_{10} - c_{11} = 0$$

Gurson yield surface: $\left(\frac{\sigma_{vm}}{\sigma_y}\right)^2 + 2f\cosh\left(\frac{3\sigma_h}{2\sigma_y}\right) - 1 - f^2 = 0$

Physics-based Derivation Before GPSR (P-GPSR)

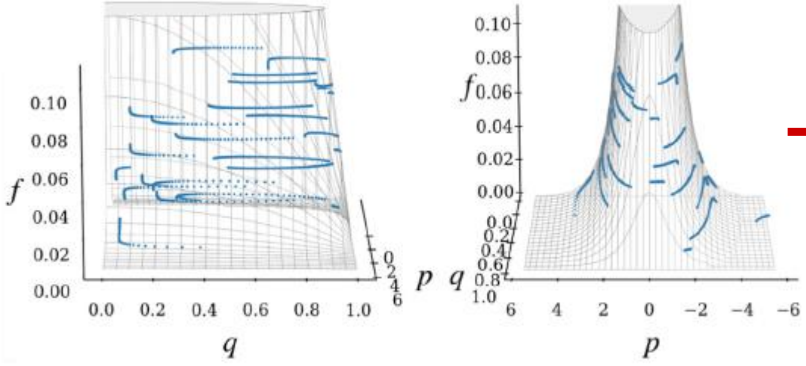
Objective: balance foundation from analytical methods with accuracy from ML

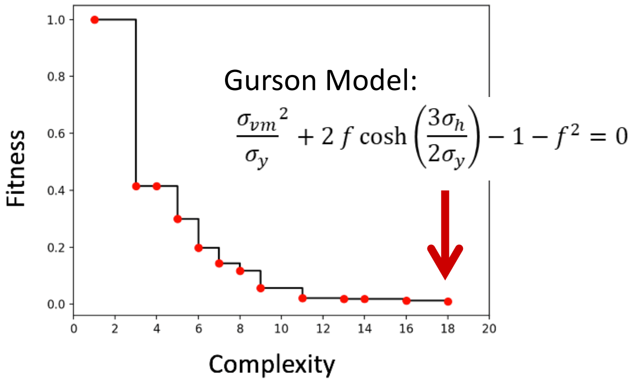
Derivation → Generate Data → Data+IML



Verification of IML Constitutive Models

- 25 load cases for training
- Gurson material model generated data



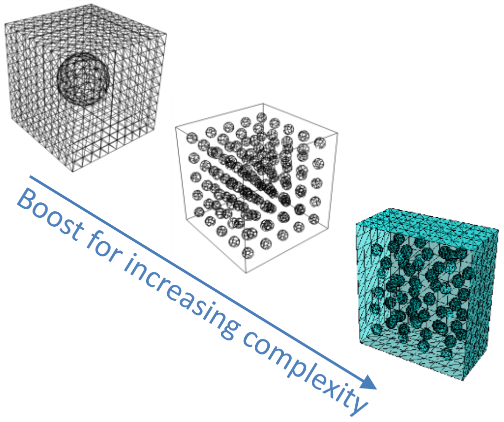


Algorithm	Generations	Median MAE	[*min*, *max*] MAE	Time (h)
GPSR	10000	$1.3\text{x}10^{-3}$	[$4.9\text{x}10^{-6}$, inf]	7
P-GPSR	250	$1.2\text{x}10^{-9}$	[<$1\text{x}10^{-20}$, $3\text{x}10^{-6}$]	1

(top) Zamora, 2022, MS Thesis, U. Utah

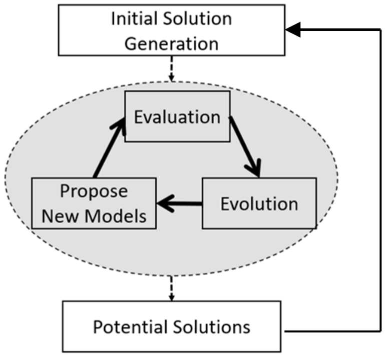
(bottom) K. Garbrecht et al., 2023, JMPS

Assumption Relaxation



$$q^2 + 2f\Theta(p,q) - 1 - f^2\Omega(p,q)$$ (without microstructure assumptions)

Assumption	Model
Void interaction	Single void, periodic BCs, void remains spherical
Void growth self similarity	Single void, periodic BCs, no void constraint



Seed Θ_i and Ω_i in initial pop. for Θ_{i+1} and Ω_{i+1}

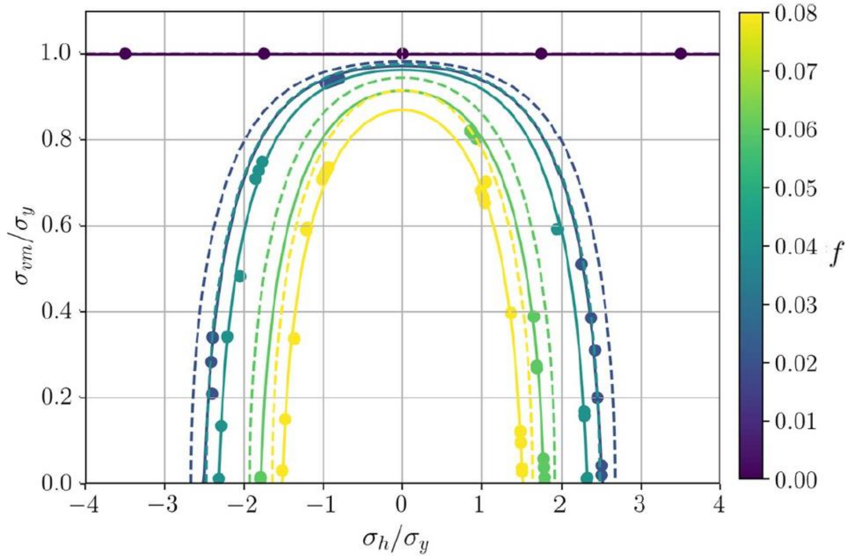
Training data and stages:

$q^2 + 2f\cosh\left(-\frac{3}{2}p\right) - 1 - f^2 1$ (with Θ_1 = $\cosh\left(-\frac{3}{2}p\right)$, Ω_1 = 1)	(with all Gurson assumptions)
$q^2 + 2f\Theta_2 - 1 - f^2\Omega_2$	(void interaction training data)
$q^2 + 2f\Theta_3 - 1 - f^2\Omega_3$	(growth self-similarity training data)

Relaxed Void Growth Self Similarity

$$q^2 + 2f\Theta(p,q) - 1 - f^2\Omega(p,q)$$

$$q^2 + 2f\left(0.1225\sqrt{q} + 1\right)\cosh\left(-\frac{3}{2}p\right) - 1 - f^2\left(\frac{\sqrt{q}}{4f} - \frac{3}{8f} - 1\right)$$



- - - - Gurson model
——— Bingo model
• Training data

Yield Surface Mapping using TTM

Mapping relies on the **tensor-transform method (TTM)**, which represents yield surfaces as:

$$\vec{\boldsymbol{\sigma}}^T \boldsymbol{P} \vec{\boldsymbol{\sigma}} = \sigma_i P_{ij} \sigma_j = 1$$

$$\vec{\boldsymbol{\sigma}}^T = [\,\sigma_1, \sigma_2, \sigma_3]$$

e.g., von Mises yield criterion:

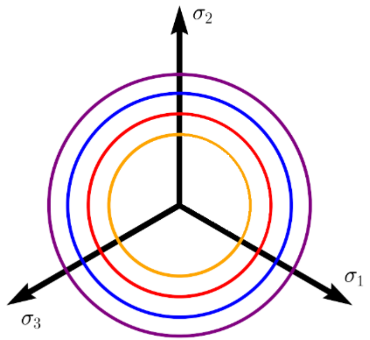
$$(\sigma_1 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2 + (\sigma_2 - \sigma_3)^2 = 2\sigma_y^2$$

$$\boldsymbol{P} = \frac{1}{\sigma_y^2}\begin{bmatrix} 1 & -1/2 & -1/2 \\ -1/2 & 1 & -1/2 \\ -1/2 & -1/2 & 1 \end{bmatrix}$$

TTM relies on **transforming a surrogate *P* tensor** via:

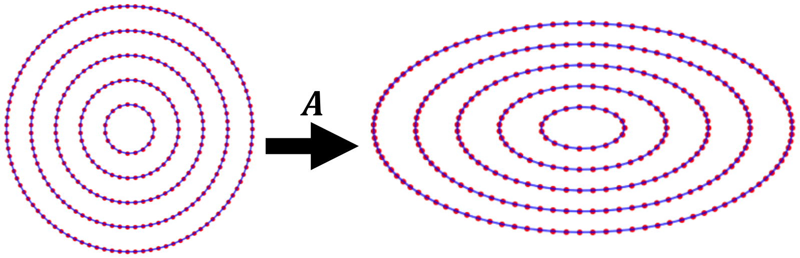
$$\boldsymbol{P}_{real} = \boldsymbol{A}^T \boldsymbol{P}_{surrogate} \boldsymbol{A}$$

$$\vec{\boldsymbol{\sigma}}^T \boldsymbol{A}^T \boldsymbol{P}_{surrogate} \boldsymbol{A} \vec{\boldsymbol{\sigma}} = 1$$



von Mises yield surface projection on the **deviatoric plane represents a circle**

This is our **surrogate (isotropic) yield surface**



Training Data Generation: VPSC

- Each grain is a visco-plastic anisotropic ellipsoidal inclusion that has a deviatoric plastic response within a visco-plastic anisotropic Homogeneous Effective Medium (HEM).
- Stress and strain are uniform within a grain (inclusion) but can differ from the HEM values, in contrast to a Taylor model (where strain rates are equivalently imposed).

Grain strain rate is a sum slip rate on each system, s, obtained by the Schmid tensor, m, and stresses σ, τ^s → $$\dot{\varepsilon}_{ij}' = \dot{\gamma}_o \sum_s m_{ij}^s \left(\frac{m^s : \sigma}{\tau^s}\right)^n = M_{ijkl}\sigma_{kl}'$$

The HEM is subject to an equivalent strain rate where an interaction tensor, M, describes the 'stiffness' → $$\overline{\dot{\varepsilon}_{ij}}' = \overline{M}_{ijkl}\overline{\sigma}_{kl}'$$

Equilibrium is enforced by solving stress divergence equation (conservation of momentum): → $$\sigma_{ij,j} = \left(\sigma_{ij}' + p\delta_{ij}\right)_{,j} = 0$$

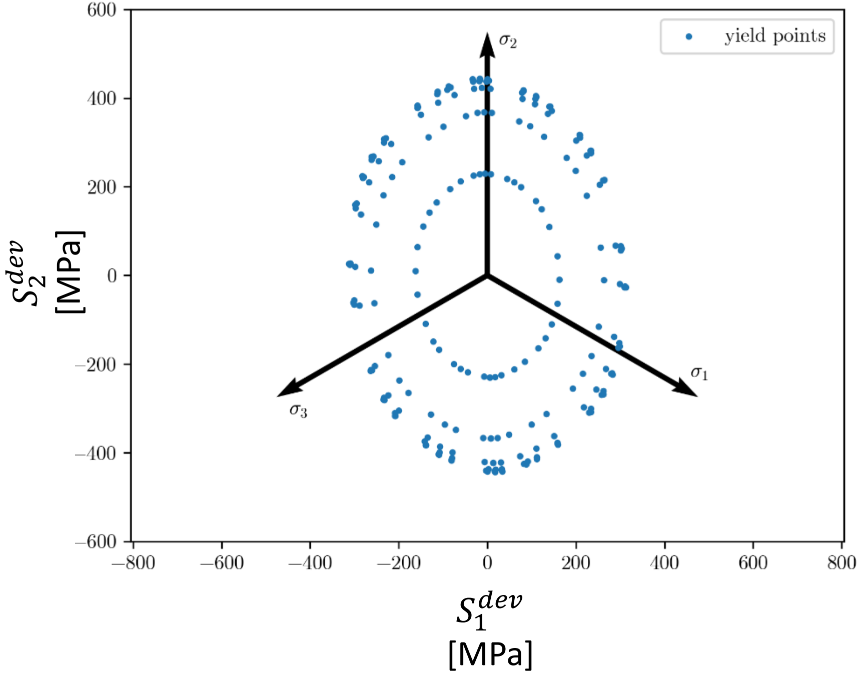
Yield Surface Mapping using TTM

Yield surfaces **representing highly textured stainless steel** were generated with **VPSC** (i.e., simulated data)

Objective: demonstrate the ability to map arbitrary yield surfaces to surrogates

Training data:

- Stainless steel loaded with $\epsilon_{vm} \in [0, 0.125]$
- Yield surfaces extracted at 6 points during loading history
- 37 points per ϵ_{vm} value

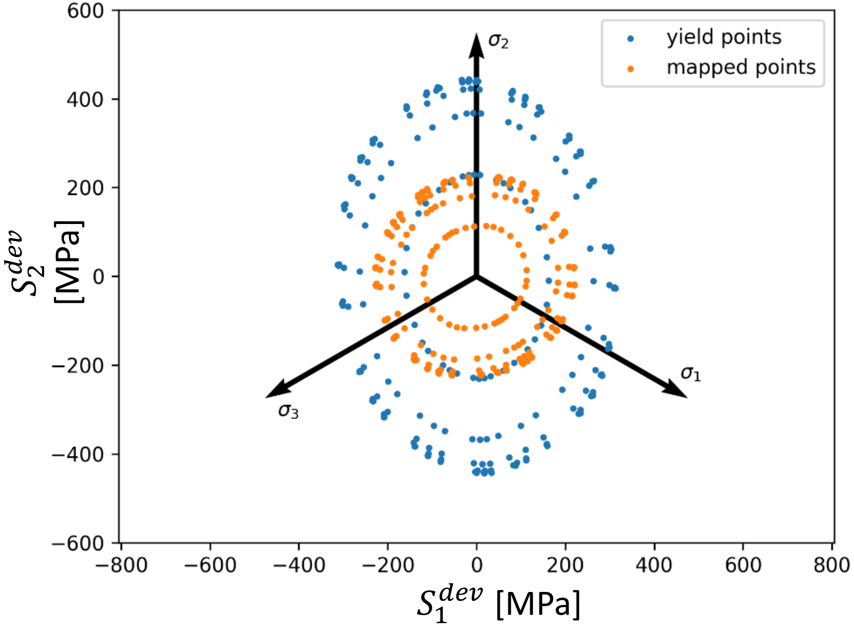


Yield Surface Mapping using TTM

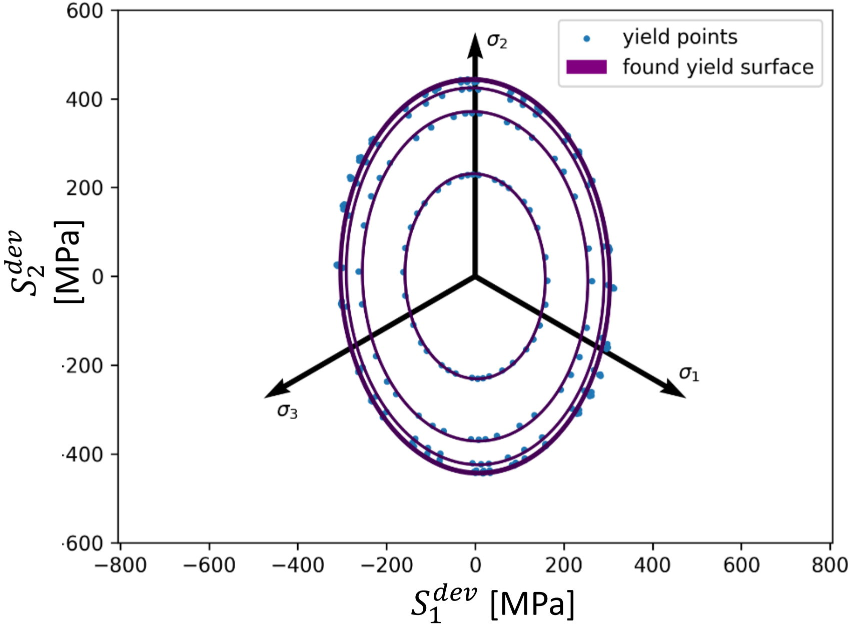
$$\boldsymbol{B} = \boldsymbol{A}^{-1} = (0.000228\epsilon_{vm} + 5.298)\begin{bmatrix} -0.225 & 0.39 & 0.23 \\ -0.093 & 0.41 & 0.075 \\ -0.258 & 0.512 & 0.139 \end{bmatrix}$$

MSE = 0.0108

Apply $\boldsymbol{B}$ to training data



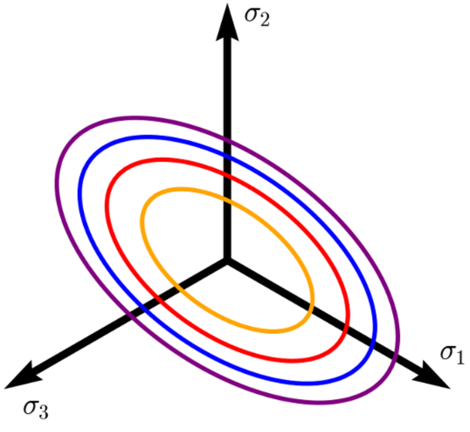
Apply $\boldsymbol{A}$ to surrogate surface



Department of
MECHANICAL ENGINEERING
THE UNIVERSITY OF UTAH

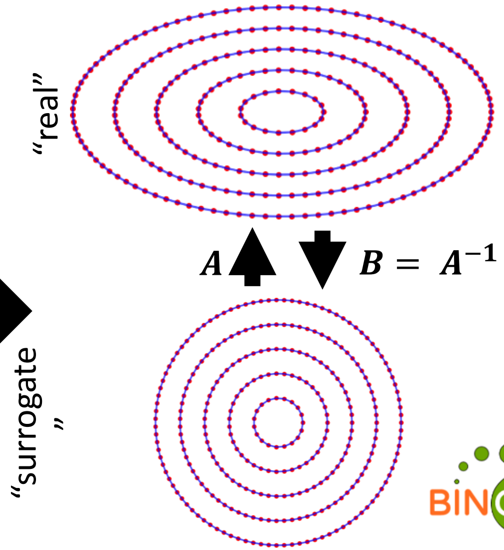
Finite Element Method Auto-implementation

Data collection



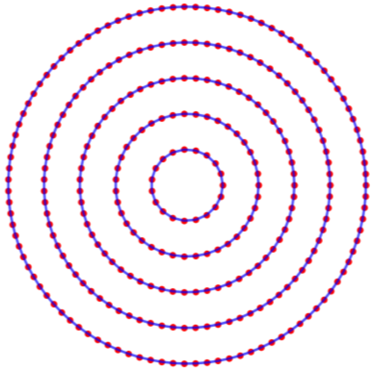
Collect yield-surface data, typically from experiment ("real")

Map to surrogate yield surface



Use IML to find mapping tensor $\boldsymbol{A}$ from "real" (anisotropic) surface to a surrogate (isotropic) surface similar to *Oller et al.

Solve FE model with surrogate model



Solve finite-element model with a single surrogate implemented as a user constitutive model (e.g., UMAT in ABAQUS)

Summary

1. Interpretable, Data-driven Machine Learning Background

- We seek interpretable and generalizable material constitutive models
- GPSR provides one means for inherent interpretability through the evolution of analytical expressions
- A purely data-driven approach results in accurate but unclear models

2. Laying a Scientific Machine Learning Foundation

- Partial derivation before the ML process:
  - forms a guiding parent equation
  - improves model accuracy and training performance
  - define features of importance in training data sets, and
  - promotes generalizable models
- Verification studies (i.e., checking for known analytical models) with GPSR are a natural step
- Microstructure complexity can be added iteratively to produce an accurate, complex, but still interpretable model

3. Finite Element Method Auto-implementation

- With the tensor transform method, only one surrogate constitutive model need be implemented in FEA and GPSR provides the transform to the real constitutive model