Surrogate models of elastic responses from truss lattices for multiscale design

WCSMO 14

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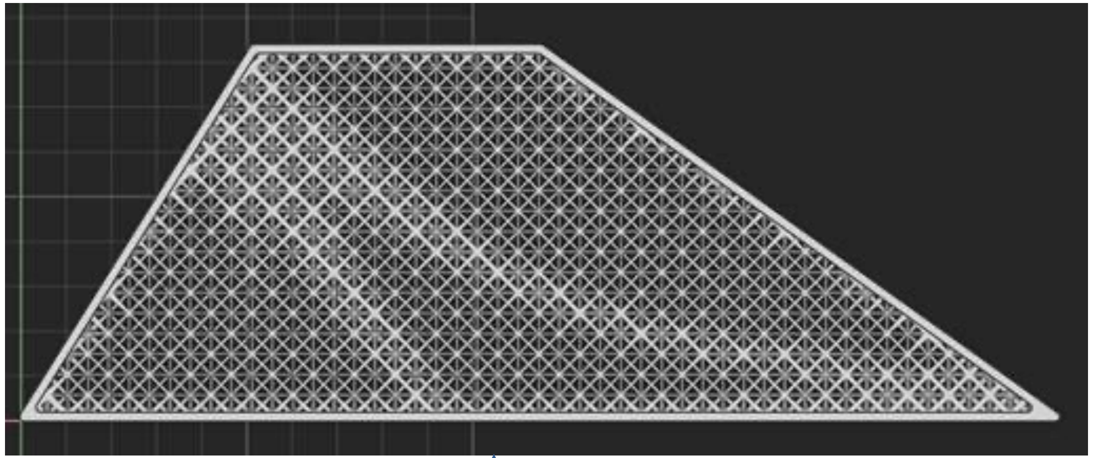
Using surrogate models for linear elastic material models and concerned whether stiffness tensors are positive definite

- Interested in design optimization of functionally graded materials
- Using surrogate models to represent homogenized micro truss structures
- Show an example where surrogate stiffness tensors are not positive definite
- Discuss a few approaches to obtain positive definite stiffness tensors
- Propose positive definite model validation as an optimization problem

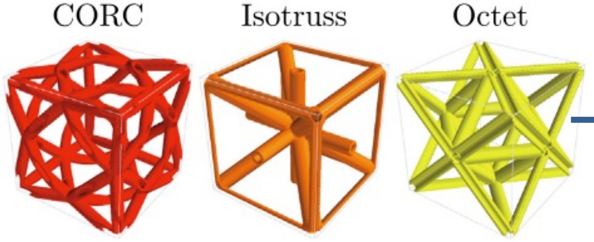
Surrogate models for micro-architected materials

- Learning the homogenized stiffness tensors of various hollow lattice architectures [1] [2]
- Density based topology optimization to design functionally graded micro-geometry
- Design variables are cylindrical rod diameters
- **Surrogate model** to represent homogenized material
  - Outputs stiffness tensors as function of rod diameters
  - Differentiable with respect to design variables

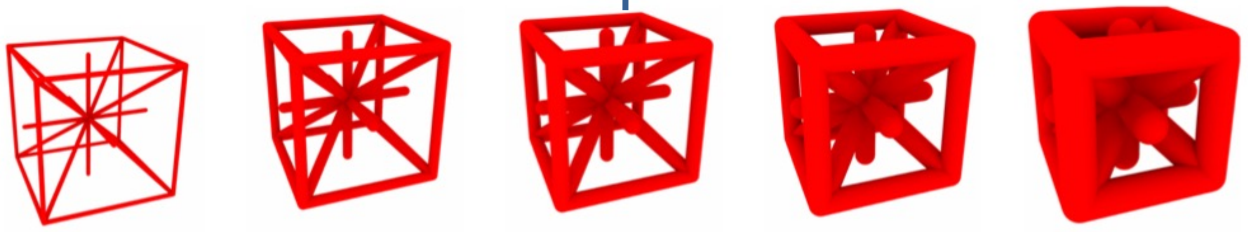


Functionally Graded Optimal Design

Various Lattices



Design Range



Learning the homogenized stiffness tensors from data

- Model learns $\boldsymbol{C}$ as function of
  - Inner radius to outer radius ratio ι
  - Outer rod radius r
  - Poisson's ratio ν
- Required to produce all derivatives
  - $\frac{\partial \boldsymbol{C}}{\partial \iota}, \frac{\partial \boldsymbol{C}}{\partial r}, \frac{\partial \boldsymbol{C}}{\partial \nu}$
- 21 coefficients to learn for anisotropy
- 9 coefficients to learn for orthotropy
  - Reasonable if using 1/8 symmetry

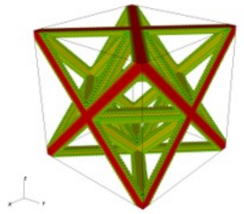
Anisotropic

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{13}\\ \sigma_{12}\end{bmatrix} = \begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & C_{1123} & C_{1113} & C_{1112}\\ & C_{2222} & C_{2233} & C_{2223} & C_{2213} & C_{2212}\\ & & C_{3333} & C_{3323} & C_{3313} & C_{3312}\\ & & & C_{2323} & C_{2313} & C_{2312}\\ & & symm & & C_{1313} & C_{1312}\\ & & & & & C_{1212}\end{bmatrix} \begin{bmatrix}\epsilon_{11}\\ \epsilon_{22}\\ \epsilon_{33}\\ 2\epsilon_{23}\\ 2\epsilon_{13}\\ 2\epsilon_{12}\end{bmatrix}$$

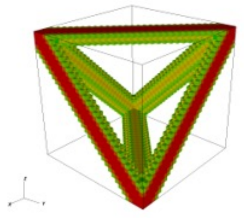
Orthotropic

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{13}\\ \sigma_{12}\end{bmatrix} = \begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & 0 & 0 & 0\\ C_{1122} & C_{2222} & C_{2233} & 0 & 0 & 0\\ C_{1133} & C_{2233} & C_{3333} & 0 & 0 & 0\\ 0 & 0 & 0 & C_{2323} & 0 & 0\\ 0 & 0 & 0 & 0 & C_{1313} & 0\\ 0 & 0 & 0 & 0 & 0 & C_{1212}\end{bmatrix} \begin{bmatrix}\epsilon_{11}\\ \epsilon_{22}\\ \epsilon_{33}\\ 2\epsilon_{23}\\ 2\epsilon_{13}\\ 2\epsilon_{12}\end{bmatrix}$$

Octet Truss

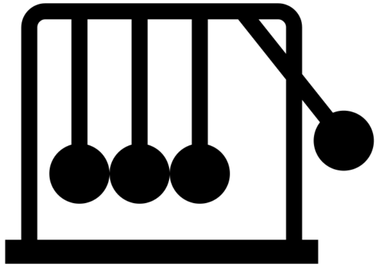


1/8th Symmetric Octet Truss



Surrogate model needs to produce positive definite stiffness tensors

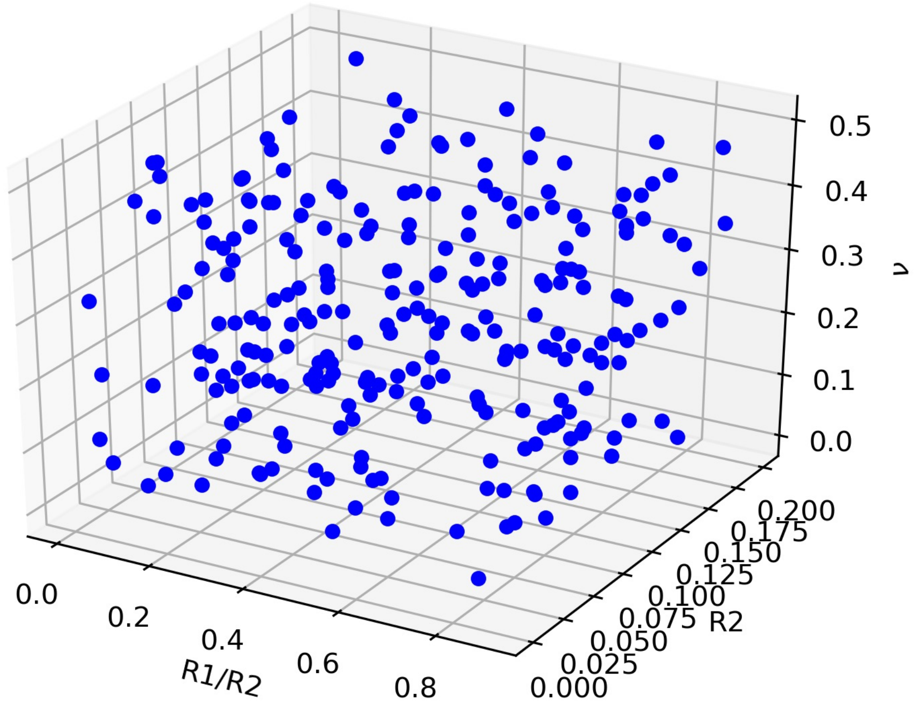
- Stiffness tensor $\boldsymbol{C}$ must be positive definite
- Ensure uniqueness of PDE
- Required for strain energy to be positive
  - Materials generally store energy when deformed
  - If positive definite is violated, the material releases energy when deformed



The surrogate models must obey physics,
but is this really a problem?

Investigation on whether we need to be concerned about positive definite surrogate predictions

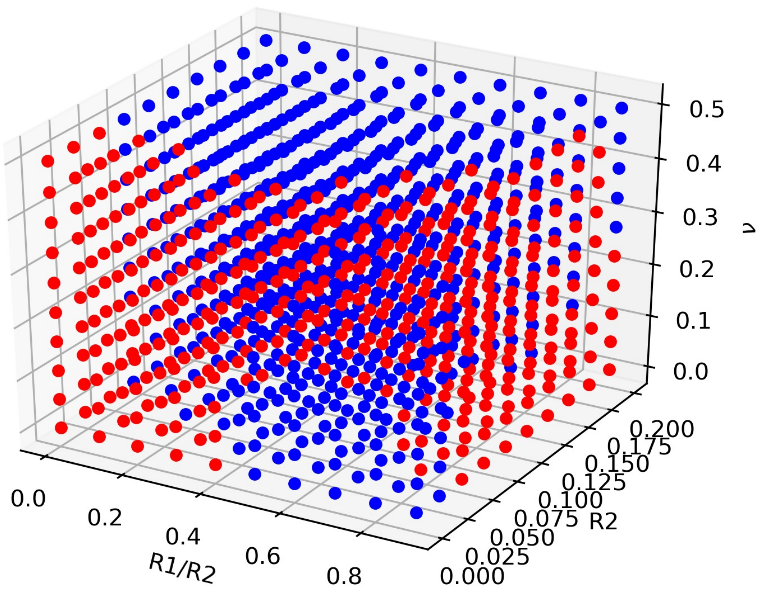
- Homogenized dataset from hollow strut Octet truss
- 250 Data points in 3 dimensions
  - Random Latin Hypercube sampling
  - Input dimensions: radius ratio, outer radius, Poisson's ratio
- All homogenized stiffness tensors are positive definite!
  - Our homogenization solver obeys physics!
- Train various surrogate models to this data
  - Evaluate the trained models on factorial design
  - Show examples where the surrogate stiffness tensor is not positive definite



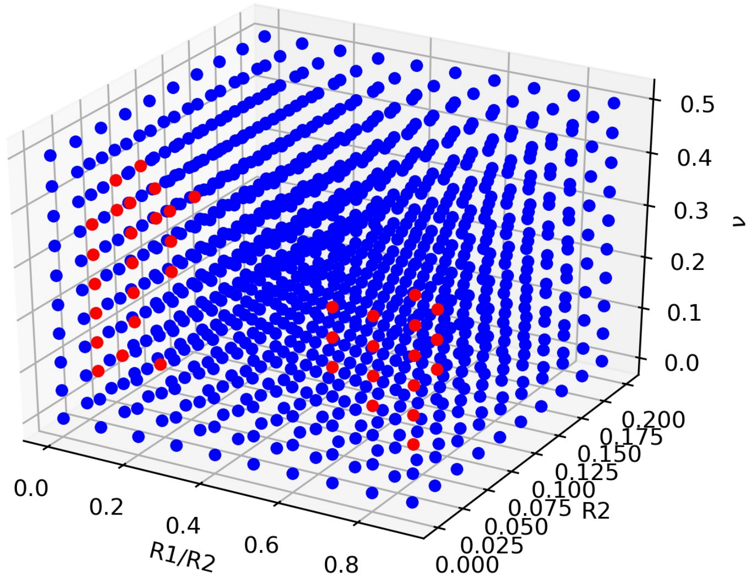
Surrogate stiffness tensors were not positive definite on the domain!

- Red points are not positive definite
- **Blue** points are positive definite

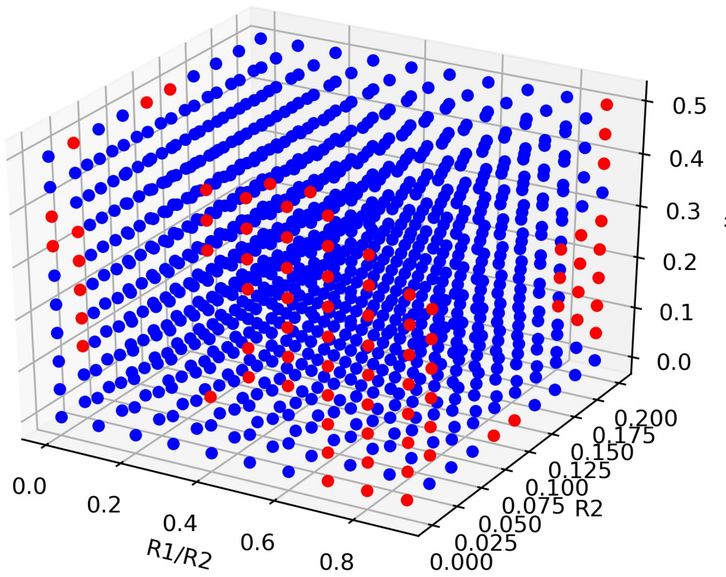
Quadratic Polynomial



Linear Kernel Radial Basis Functions



Neural Network



Training to positive definite data does not guarantee positive definite predictions.

Approaches we can take to achieve positive definite stiffness tensors

- Data driven approach and build a larger dataset
- Use specialized loss functions to penalize non-positive definite data points
- Prove that a surrogate model architecture will always be positive definite
- Manually iterate architectures with numerical validation

Why we are showing our numerical validation approach

- Data driven approach and build a larger dataset
  - It is not known how much data you will need
  - Extra homogenization simulations incurs additional cost
- Use specialized loss functions to penalize non-positive definite data points
  - This only enforces positive definiteness at point locations
  - Does not enforce on the entire domain!
- Prove that a surrogate model architecture will always be positive definite
  - Does not generalize to arbitrary surrogate models
  - Do we make sacrifices in potential model accuracy?
- Manually iterate architectures with numerical validation
  - **We need to validate our surrogate models anyways!**

Sylvester's criteria is commonly used to outline material stability

- Sylvester's criteria states that $\boldsymbol{C}$ is positive-definite if and only if all of the following have a positive determinant:
  - the upper left 1-by-1 corner of $\boldsymbol{C}$
  - the upper left 2-by-2 corner of $\boldsymbol{C}$
  - the upper left 3-by-3 corner of $\boldsymbol{C}$
  - the upper left 4-by-4 corner of $\boldsymbol{C}$
  - the upper left 5-by-5 corner of $\boldsymbol{C}$
  - $\boldsymbol{C}$ itself.
- Commonly used to define material model coefficient stability
- We need to ensure Sylvester's criteria is satisfied on the entire design domain!

Derivative information is available from our surrogate models

- Predictions for $\boldsymbol{C}$ are generated in a machine learning framework
- Use automatic differentiation of these predictions to get derivative information
- Easily compute derivatives of Sylvester's criteria!
- Sounds like an optimization problem
  - Want to find the smallest values in a domain
  - If the smallest values are positive, then our model is positive definite
  - Derivative information is available

$$\frac{\partial(\mathbf{det}\,\boldsymbol{C}(\iota, r, \nu))}{\partial \iota}$$

$$\frac{\partial(\mathbf{det}\,\boldsymbol{C}(\iota, r, \nu))}{\partial r}$$

$$\frac{\partial(\mathbf{det}\,\boldsymbol{C}(\iota, r, \nu))}{\partial \nu}$$

Positive definite validation as an optimization problem

- Find the minimum of the six determinants on the design domain
  - Use multi-start gradient based optimization
  - Start from random points on the design domain
- **If any minimum is less than zero, then model is not positive definite!**
- Number of optimizations performed dictates certainty of finding the lowest possible value
- With three input dimensions, 100 L-BFGS-B optimizations seemed sufficient
  - Very cheap to perform, results almost instantaneous!

1) Minimize $\det \boldsymbol{C}_{1x1}\ (\iota, r, \nu)$

2) Minimize $\det \boldsymbol{C}_{2x2}\ (\iota, r, \nu)$

3) Minimize $\det \boldsymbol{C}_{3x3}\ (\iota, r, \nu)$

4) Minimize $\det \boldsymbol{C}_{4x4}\ (\iota, r, \nu)$

5) Minimize $\det \boldsymbol{C}_{5x5}\ (\iota, r, \nu)$

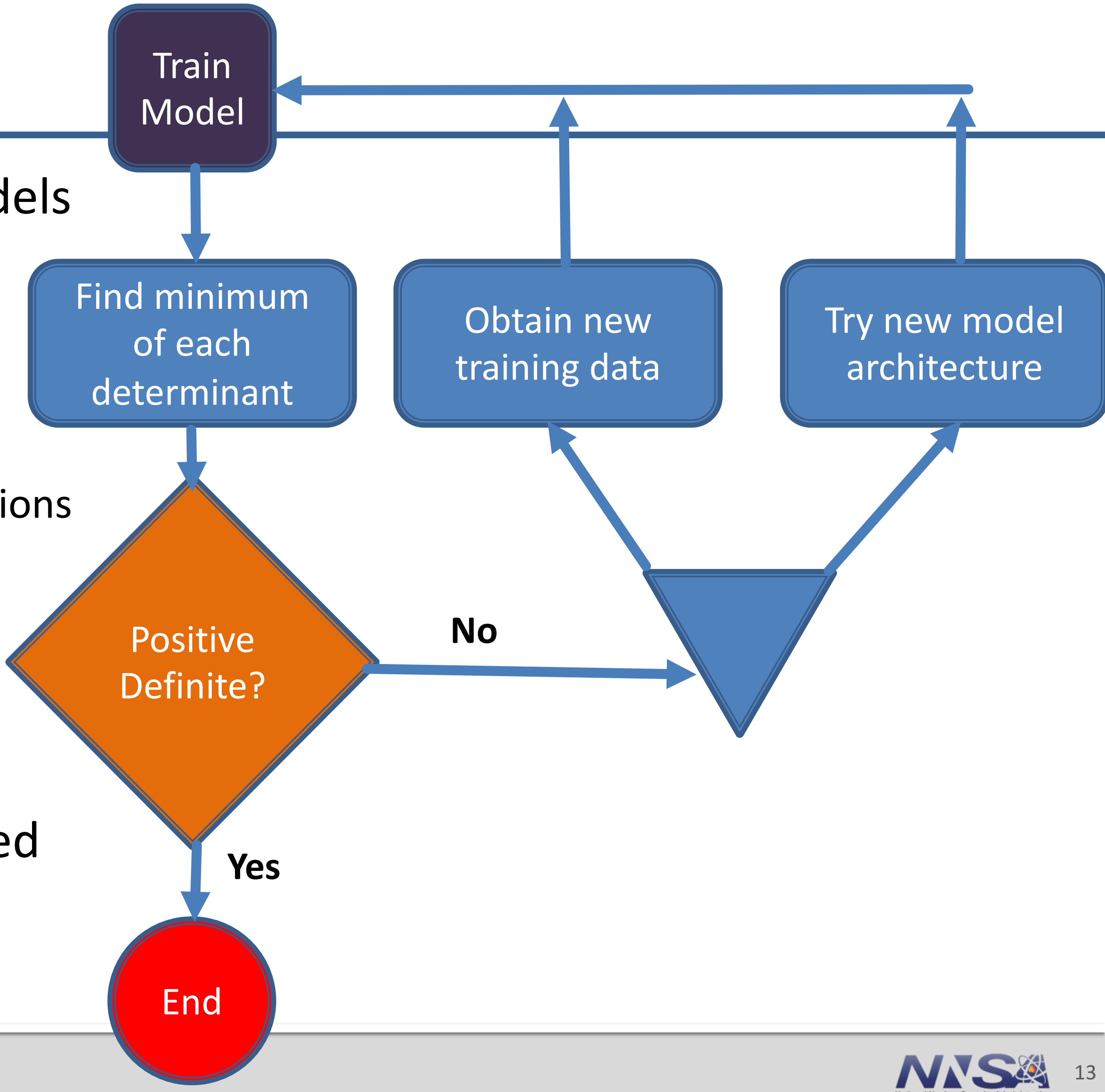
6) Minimize $\det \boldsymbol{C}(\iota, r, \nu)$

Subject to:

$$\iota_l \leq \iota \leq \iota_u$$
$$r_l \leq r \leq r_u$$
$$\nu_l \leq \nu \leq \nu_u$$

Our validation process

- It is very easy to generate surrogate models that are not physical!
- For orthotropic material models
  - Ensure most coefficients are positive
  - Can be enforced with simple activation functions
- Take hints from which determinants fail
  - Restrict the architecture in these regions
  - Or add more data in these locations!
- Our implementation has been generalized for arbitrary anisotropic models



Conclusions

- Using surrogate models to learn homogenized stiffness tensors of various hollow lattice architectures
  - These surrogate models are then used to design functionally graded materials
  - Material models can be non-linear with respect to lattice geometry
- The surrogate stiffness tensors must be positive definite
  - Chances of generating non-positive definite surrogates
  - Discussed various methods to ensure model obeys physics
- Demonstrated an optimization framework to validate surrogate models
  - Find the minimum of Sylvester's criteria over the domain
  - Computationally efficient derivative information is available
- Future work
  - Physics informed adaptive sampling training process
  - Finding classes of models that will always be positive definite
  - Introducing loss functions that prioritize positive definite constraints

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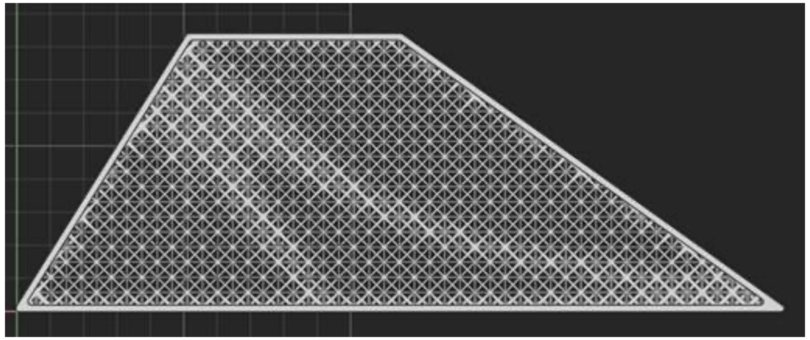
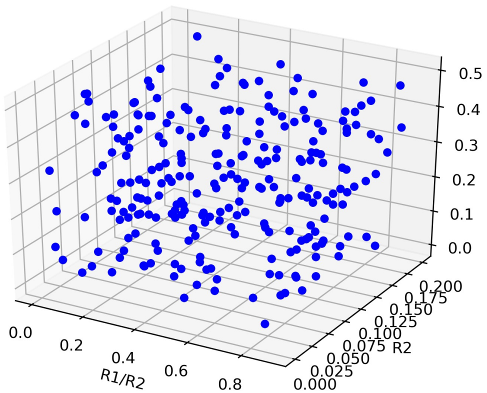
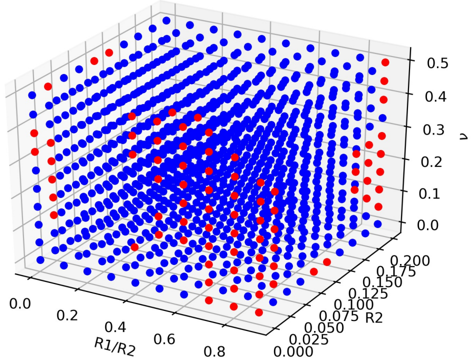
Designing functionally graded parts using homogenized material models



Positive definite training data may not be enough!

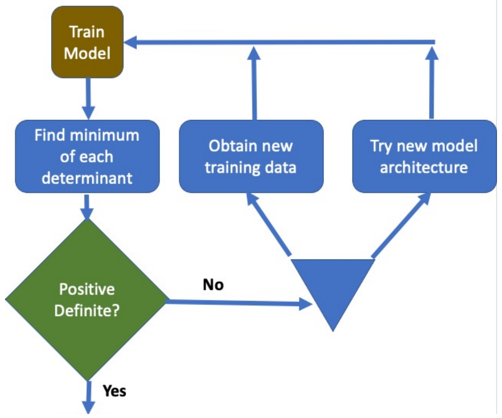




Sylvester's criteria as optimization problem to validate surrogate models

1) Minimize **det** $\boldsymbol{C}_{1x1}$ (ι, r, ν), 2) Minimize **det** $\boldsymbol{C}_{2x2}$ (ι, r, ν), 3) Minimize **det** $\boldsymbol{C}_{3x3}$ (ι, r, ν), 4) Minimize **det** $\boldsymbol{C}_{4x4}$ (ι, r, ν), 5) Minimize **det** $\boldsymbol{C}_{5x5}$ (ι, r, ν), 6) Minimize **det** $\boldsymbol{C}(\iota, r, \nu)$

Adaptative validation process ensures surrogate model is positive definite on domain!



References

- [1] Watts, S., Arrighi, W., Kudo, J. *et al.* Simple, accurate surrogate models of the elastic response of three-dimensional open truss micro-architectures with applications to multiscale topology design. *Struct Multidisc Optim* **60,** 1887–1920 (2019). https://doi.org/10.1007/s00158-019-02297-5

- [2] Watts, S., 2020. Elastic response of hollow truss lattice micro-architectures. *International Journal of Solids and Structures*, *206*, pp.472-564. https://doi.org/10.1016/j.ijsolstr.2020.08.018.

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