Data-driven constitutive laws for hyperelasticity in principal space: mechanical challenges and remedies

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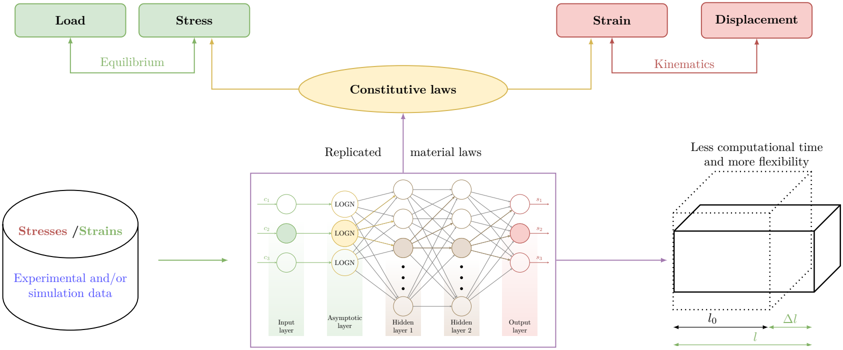
Introduction | Constitutive modelling



Hyperelasticity in principal space | Physical constraints

The constitutive relation should obey physical consistency requirements (Ogden 1997; Klein et al. 2022), namely:

1. Material frame indifference.
2. Material symmetry transformation.
3. Normalization: $\boldsymbol{s}(\boldsymbol{c} = \boldsymbol{I}) = 0$.
4. Growth conditions: asymptotic behavior.
5. The relationship of $\boldsymbol{s}(\boldsymbol{c})$ is monotonically nondecreasing.
6. The derivative $\frac{\partial \boldsymbol{s}(\boldsymbol{c})}{\partial \boldsymbol{c}}$ is positive semi-definite.

The ANN based constitutive relation should fulfill these requirements. It is a challenge.

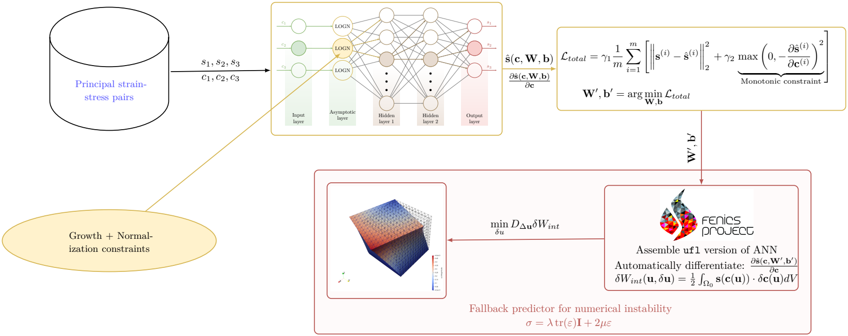
ANN based constitutive laws | Challenges

However, in practise, the "naive" ANN as material law in FEM tasks, could likely experiences:

- Numerical instability: divergent behaviour of the Newton-Raphson procedure.
- Local strain extrema: out-of-training range during the Newton-Raphson iterations.
- Non-zero stress state in the undeformed configuration.

E.g. Fuhg, Marino, and Bouklas (2022) also reported these behaviours listed above.

ANN based constitutive laws | schematic diagram



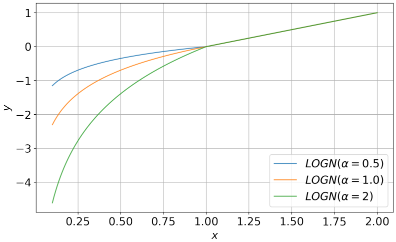
- Principal strain/stress as inputs/outputs: fulfill 1, 2 conditions.
- Asymptotic layer guarantees 3 growth, 4 normalization constraints.
- Imposed 5 monotonicity weakly in Loss function.
- Employ consistency condition of isotropic hyperelasticity as fallback predictor.

ANN based constitutive laws | Remedies I

Logarithmic neuron `LOGN()`, a new activation function (motivated from `ReLU`):

$$\texttt{LOGN(x)} = \begin{cases} \alpha \ln[x + 10^{-6}] & \text{if } x < 1.0, \\ x - 1.0 & \text{otherwise.} \end{cases} \quad (1)$$

Where α : trainable parameter.



LOGN *with various* α*.* α *controls the "strength" of the asymptotes*

ANN based constitutive laws | Remedies II

Violation of requirements 5 of $\boldsymbol{s}(\boldsymbol{c})$, 6 of the $\frac{\partial \boldsymbol{s}(\boldsymbol{c})}{\boldsymbol{c}}$ may lead to local strain extrema and numerical instability.

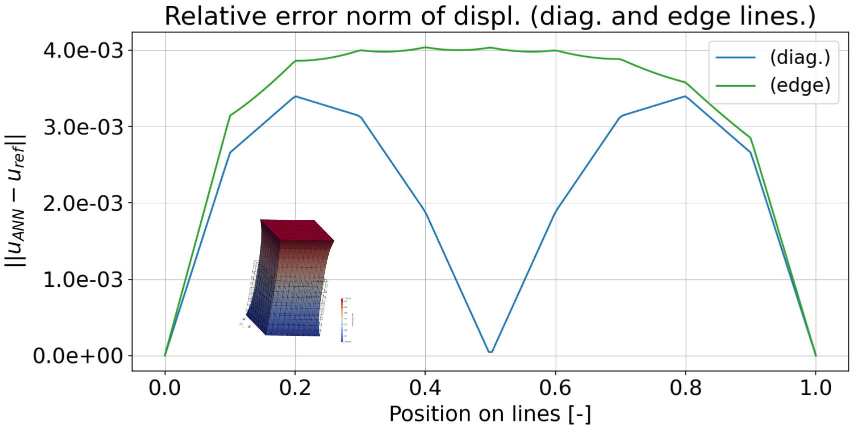
Hence, in the out-of-training regime, any funtion that fulfills 5, 6 constraints can be used as a fallback predictor. One choice is:

$$s_i^{fallback}(c_i) = \left[\frac{\lambda}{2}(c_1 + c_2 + c_3 - 3) - \mu\right] + \mu c_i,$$

where λ, μ : Lamé constants.

In this work, fallback predictor is only applied on 3 times outside the training range.

Results | Neo-Hookean Model vs ANN I

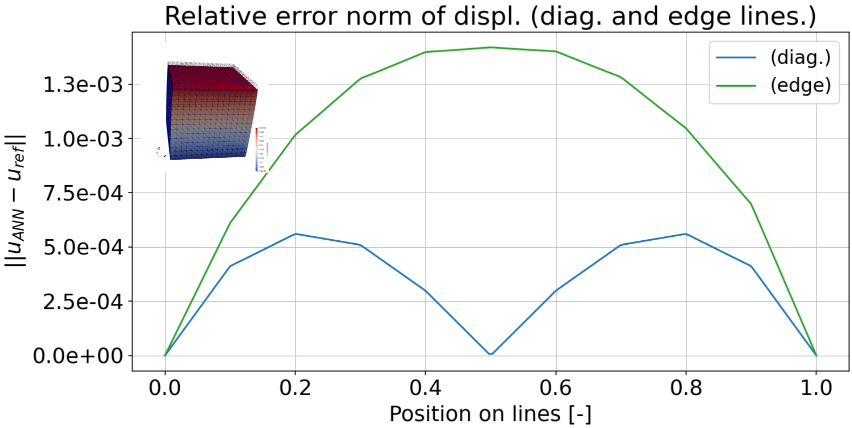


Comparison of displ. lines between ANN vs FEM (spectral forms). Uni-axial extension at 75% (no stepping).

Relative error norm over all domain: $\frac{||\mathbf{u}_{ANN} - \mathbf{u}_{ref}||}{||\mathbf{u}_{ref}||} = 7.025e - 03$

Line coor.: Diag.: $A(0,0,0) - B(1,1,1)$*; edge:* $A(1,1,0) - B(1,1,1)$

Results | Neo-Hookean Model vs ANN II

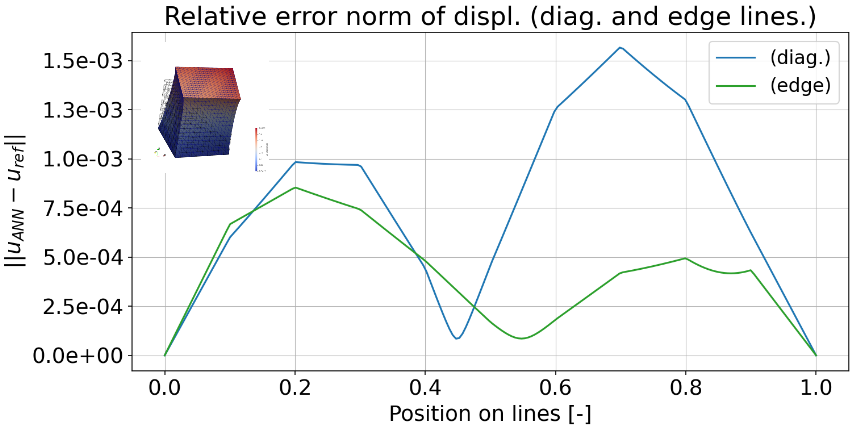


Comparison of displ. lines between ANN vs FEM (spectral forms). Uni-axial compression at 5% (no stepping).

Relative error norm over all domain: $\frac{||\mathbf{u}_{ANN} - \mathbf{u}_{ref}||}{||\mathbf{u}_{ref}||} = 1.96e - 02$

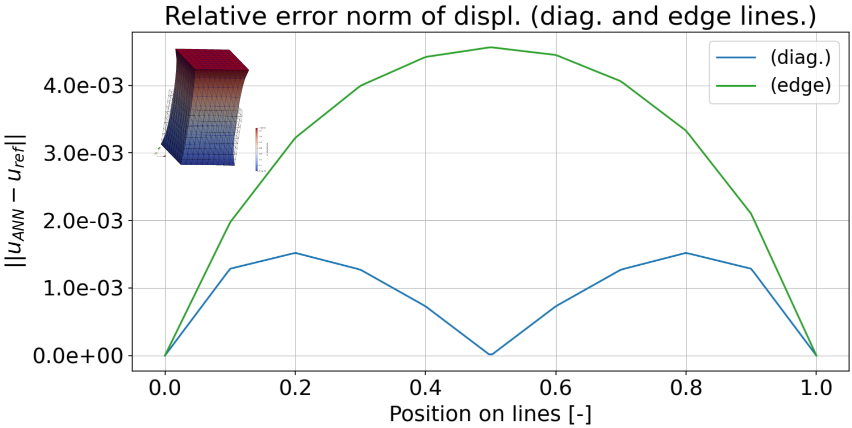
Line coor.: Diag.: $A(0,0,0) - B(1,1,1)$*; edge:* $A(1,1,0) - B(1,1,1)$

Results | Neo-Hookean Model vs ANN III



Comparison of displ. lines between ANN vs FEM (spectral forms). Uni-axial extend. 50% *and rotation about z-axis* 10° *simultaneously (no stepping).*
Relative error norm over all domain: $\frac{||\boldsymbol{u}_{ANN} - \boldsymbol{u}_{ref}||}{||\boldsymbol{u}_{ref}||} = 3.762e - 03$
Line coor.: Diag.: $A(0,0,0) - B(1,1,1)$; *edge:* $A(1,1,0) - B(1,1,1)$

Results | Ogden (3 paramters) model vs ANN I

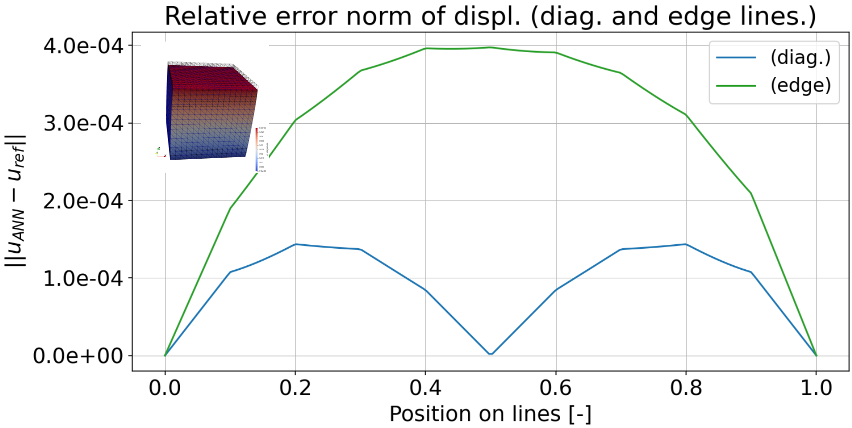


Comparison of displ. lines between ANN vs FEM (spectral forms). Uni-axial extension at 75% (no stepping).

Relative error norm over all domain: $\frac{||\boldsymbol{u}_{ANN} - \boldsymbol{u}_{ref}||}{||\boldsymbol{u}_{ref}||} = 4.358e - 03$

Line coor.: Diag.: $A(0,0,0) - B(1,1,1)$*; edge:* $A(1,1,0) - B(1,1,1)$

Results | Ogden (3 paramters) model vs ANN II

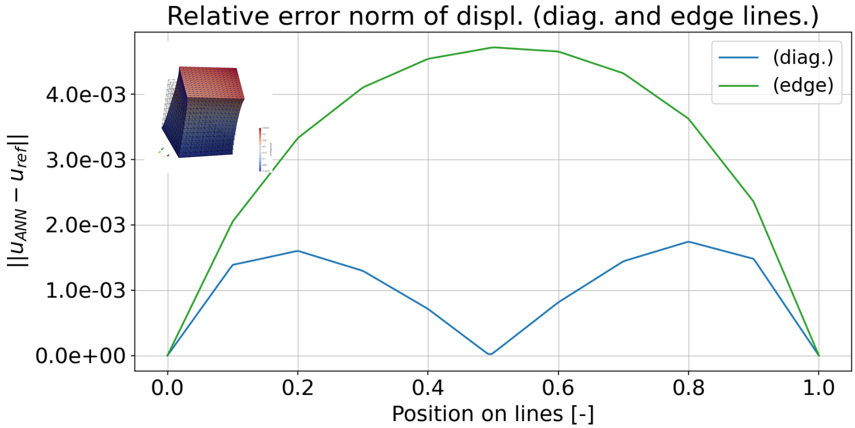


Comparison of displ. lines between ANN vs FEM (spectral forms). Uni-axial compression at 5% (no stepping).

Relative error norm over all domain: $\frac{||\boldsymbol{u}_{ANN} - \boldsymbol{u}_{ref}||}{||\boldsymbol{u}_{ref}||} = 5.565e-03$

Line coor.: Diag.: $A(0,0,0) - B(1,1,1)$*; edge:* $A(1,1,0) - B(1,1,1)$

Results | Ogden (3 paramters) model vs ANN III



Comparison of displ. lines between ANN vs FEM (spectral forms). Uni-axial extend. 50% and rotation about z-axis 10° simultaneously (no stepping).

Relative error norm over all domain: $\frac{||\mathbf{u}_{ANN} - \mathbf{u}_{ref}||}{||\mathbf{u}_{ref}||} = 7.157e - 03$

Line coor.: Diag.: $A(0,0,0) - B(1,1,1)$*; edge:* $A(1,1,0) - B(1,1,1)$

Summary

This research in 30s

- Hyperelastic material laws are learnt from strain-stress datasets in principal space using ANN.
- New activation function, modified loss are employed to satisfy normalization, asymptotic, and monotonic behaviours of the material laws.
- Fallback predictor proved helpful to avoid numerical instability in certain cases of local strain extrema.
- The ANN expression is then used within the FEniCS framework for numerical prediction of stresses fields at extreme cases.

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https://driven.uni.lu

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Fonds National de la Recherche Luxembourg

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[2] Dominik K Klein et al. “Polyconvex anisotropic hyperelasticity with neural networks”. In: *Journal of the Mechanics and Physics of Solids* 159 (2022), p. 104703.

[3] Jan N Fuhg, Michele Marino, and Nikolaos Bouklas. “Local approximate Gaussian process regression for data-driven constitutive models: development and comparison with neural networks”. In: *Computer Methods in Applied Mechanics and Engineering* 388 (2022), p. 114217.