


Data-driven hyperelastic constitutive neural network model with Laplace parameterisation

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Abstract

This paper presents a mathematical description of CLANN (Convex Laplace Artificial Neural Network), a neural model for hyperelastic materials in nonlinear continuum mechanics. The model is built on hyperelasticity, convexity, and frame invariance. A Cholesky-based logarithmic parameterization of the right Cauchy–Green tensor ensures convexity and enables stable differentiation. An input convex neural network (ICNN) with nonnegative output weights defines a strictly convex stored-energy density. Second Piola–Kirchhoff stresses are obtained by differentiating the energy with respect to the strain measure via the chain rule, which guarantees thermodynamic consistency and objective, conservative stresses. We provide explicit 2D formulas for stresses and an analytic Hessian used in Newton’s method, together with a training loss that augments data misfit with anchors at the undeformed state to enforce zero energy and zero stress. The convexity of the energy yields positive-definite tangent moduli and robust convergence, while the logarithmic parameterization handles large strains. The approach integrates efficiently with finite element solvers and recovers linear elasticity in the small-strain limit.

Keywords: hyperelasticity; convex neural networks; continuum mechanics; thermodynamics; finite elements

1. Introduction

We introduce CLANN (Convex Laplace Artificial Neural Network), a data-driven hyperelastic constitutive model for nonlinear continuum mechanics. CLANN is built on three principles: (i) hyperelasticity, where stresses are derived from a scalar stored-energy potential ψ ; (ii) strict convexity, which guarantees uniqueness, stability, and positive-definite tangent moduli; and (iii) frame invariance, achieved by defining ψ in terms of the right Cauchy–Green tensor $C = F^T F$. We parameterize C through its upper Cholesky factor and use logarithmic coordinates, which enable an input convex neural network (ICNN) to represent a strictly convex energy. Second Piola–Kirchhoff stresses and the consistent tangent are obtained by analytic differentiation via the chain rule, ensuring thermodynamic consistency and efficient finite element (FE) integration. The model handles large strains robustly and reduces to linear elasticity in the small-strain limit.

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2. Materials and Methods 30

2.1. Kinematics and Parameterization 31

Let F denote the deformation gradient and $C = F^\top F$ the right Cauchy–Green tensor. We use the upper-triangular Cholesky factor U such that $C = U^\top U$. In 2D, introduce logarithmic coordinates 32
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$$\xi_1 = \ln(u_{11}), \quad \xi_2 = \ln(u_{22}), \quad \xi_3 = \frac{u_{12}}{u_{11}}, \quad (1)$$

which improve conditioning at large strains and support convex modeling in ξ . 35

2.2. Convex Neural Energy 36

An input convex neural network defines a strictly convex energy $\psi(\xi)$: 37

$$z = \frac{\text{softplus}(\beta W_1 \xi)}{\beta}, \quad \psi = W_2^\top z + b_2, \quad (2)$$

with nonnegative output weights $W_2 \geq 0$ to preserve convexity. As a consequence, the Hessian $H = \partial^2 \psi / \partial \xi^2$ is positive definite. 38
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2.3. Stresses and Consistent Tangent 40

Hyperelastic stresses follow from the chain rule: 41

$$S = \frac{\partial \psi}{\partial C} = \frac{\partial \psi}{\partial \xi} \frac{\partial \xi}{\partial C}, \quad g = \frac{\partial \psi}{\partial \xi}. \quad (3)$$

In 2D the components admit explicit expressions 42

$$\begin{aligned} S_{11} &= e^{-2\xi_1}(g_1 - 2\xi_3 g_3) + e^{-2\xi_2} g_2 \xi_3^2, \\ S_{22} &= e^{-2\xi_2} g_2, \\ S_{12} &= -e^{-2\xi_2} g_2 \xi_3 + e^{-2\xi_1} g_3. \end{aligned} \quad (4)$$

The analytic Hessian used in Newton’s method is 43

$$H_{ij} = \frac{\partial^2 \psi}{\partial \xi_i \partial \xi_j} = \sum_h \sigma'_h w_{2,h} W_{h,i} W_{h,j}, \quad \sigma' = \beta \sigma(1 - \sigma), \quad \sigma = \text{sigmoid}(\beta s), \quad s = W_1 \xi + b_1. \quad (5)$$

2.4. Training Objective 44

Given stress data $S_{\text{exp}}^{(i)}$, the loss combines data misfit and anchors at the undeformed state: 45
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$$L = \frac{1}{N} \sum_{i=1}^N \|S_{\text{pred}}^{(i)} - S_{\text{exp}}^{(i)}\|^2 + \lambda_{SI} \|S(I)\|^2 + \lambda_{d\psi} \|\nabla_\xi \psi(0)\|^2 + \lambda_\psi \|\psi(0)\|^2. \quad (6)$$

3. Results 47

We report theoretical properties and implementation outcomes. First, strict convexity of ψ implies positive-definite tangent moduli, which enhances robustness of Newton iterations. Second, the chain-rule construction ensures objective and conservative stresses, i.e., for any closed deformation cycle the stress work vanishes. Third, the logarithmic parameterization provides symmetric behavior under tension/compression and robust handling of large strains. In the small-strain regime, CLANN reduces to linear elasticity with Lamé parameters emerging from the local quadratic approximation of ψ . 48
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3.1. Thermodynamic Consistency

Because stresses derive from an energy potential, CLANN satisfies the first law in the hyperelastic setting (no dissipation) and meets the second-law requirements for quasi-static, reversible processes. Anchors enforce $\psi(0) = 0$ and $S(I) = 0$, making the undeformed configuration an energy minimum with zero stress and vanishing gradient in ξ .

3.2. Numerical Aspects

The analytic Hessian enables consistent tangents for FE assembly and improves convergence of Newton’s method. For deployment, automatic differentiation can compute $g = \partial\psi/\partial\xi$, while closed-form expressions supply S and the tangent via $\partial\xi/\partial C$. The model can be exported to inference formats by wrapping gradient and Hessian evaluations.

4. Discussion

CLANN unifies classical hyperelastic modeling with modern convex neural networks. Compared to traditional forms (Neo-Hookean, Mooney–Rivlin, Ogden), CLANN maintains the fundamental relationship $S = \partial\psi/\partial C$ while learning ψ from data under strict convexity constraints. This yields improved stability and expressiveness, and it facilitates incorporation of priors such as near-incompressibility or anisotropy via extensions of the parameterization and network architecture. The convex design reduces non-physical responses and mitigates bifurcations in challenging loading paths.

5. Conclusions

We introduced a mathematically grounded, thermodynamically consistent neural constitutive model for hyperelasticity. A Cholesky-based logarithmic parameterization and an ICNN energy ensure strict convexity, objective stresses, and positive-definite tangents. Explicit stress and Hessian formulas support efficient FE integration and robust Newton convergence. The framework recovers linear elasticity at small strains and is well-suited to soft-tissue biomechanics; future work will address anisotropy and near-incompressibility.

6. Patents

Not applicable.

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Abbreviations

The following abbreviations are used in this manuscript:

CLANN	Convex Laplace Artificial Neural Network
ICNN	Input Convex Neural Network
FE	Finite Element
SPD	Symmetric Positive Definite
PK2	Second Piola–Kirchhoff (stress)

Appendix A

Appendix A.1

The appendix is an optional section that can contain details and data supplemental to the main text—for example, explanations of experimental details that would disrupt the flow of the main text but nonetheless remain crucial to understanding and reproducing the research shown; figures of replicates for experiments of which representative data are shown in the main text can be added here if brief, or as Supplementary Data. Mathematical proofs of results not central to the paper can be added as an appendix.

Table A1. This is a table caption.

Title 1	Title 2	Title 3
Entry 1	Data	Data
Entry 2	Data	Data

Appendix B

All appendix sections must be cited in the main text. In the appendices, Figures, Tables, etc. should be labeled, starting with “A”—e.g., Figure A1, Figure A2, etc.

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