Benchmarks for Physics-Informed Data-Driven Hyperelasticity

Workshop on Establishing Benchmarks for Data-Driven Modeling of Physical Systems

Vahidullah Tac

Kevin Linka, Francisco Sahli Costabal, Ellen Kuhl, Adrian Buganza Tepole

Purdue University

April 2023

Background

Why develop data-driven models of soft materials?

- Advanced applications in biomechanics
  - Personalized surgery
  - Medical device and procedure design
  - Thorough investigation of internal mechanisms
  - . . .
- Soft robotics
- Soft tissues and rubbers are nonlinear and undergo large deformations
- Traditional 'closed-form' material models lack flexibility
- No consensus on the choice of the best model

Background

Why develop data-driven models of soft materials?

- Advanced applications in biomechanics
  - Personalized surgery
  - Medical device and procedure design
  - Thorough investigation of internal mechanisms
  - ...
- Soft robotics
- Soft tissues and rubbers are nonlinear and undergo large deformations
- Traditional 'closed-form' material models lack flexibility
- No consensus on the choice of the best model

$\Longrightarrow$ Develop data-driven constitutive models of soft materials

Background

Why develop data-driven models of soft materials?

- Advanced applications in biomechanics
    - Personalized surgery
    - Medical device and procedure design
    - Thorough investigation of internal mechanisms
    - ...
- Soft robotics
- Soft tissues and rubbers are nonlinear and undergo large deformations
- Traditional 'closed-form' material models lack flexibility
- No consensus on the choice of the best model

$\Longrightarrow$ Develop data-driven constitutive models of soft materials

- But what about physics-based constraints?

Background

Why develop data-driven models of soft materials?

- Advanced applications in biomechanics
  - Personalized surgery
  - Medical device and procedure design
  - Thorough investigation of internal mechanisms
  - $\cdots$
- Soft robotics
- Soft tissues and rubbers are nonlinear and undergo large deformations
- Traditional 'closed-form' material models lack flexibility
- No consensus on the choice of the best model

$\Longrightarrow$ Develop data-driven constitutive models of soft materials

- But what about physics-based constraints?
  - Objectivity
  - Thermodynamic consistency
  - Polyconvexity

Physics-constrained data-driven models

Imposing physics-based constraints has several advantages:

- Physically realistic predictions
- Prevents overfitting
- Better extrapolation
- Fewer training data points required $\rightarrow$ "Learning from physics"
- Better integration into Newton-type solvers like FEM

Physics-constrained data-driven models

Imposing physics-based constraints has several advantages:

- Physically realistic predictions
- Prevents overfitting
- Better extrapolation
- Fewer training data points required $\rightarrow$ "Learning from physics"
- Better integration into Newton-type solvers like FEM

Choices for imposing physics-based constraints:

Physics-constrained data-driven models

Imposing physics-based constraints has several advantages:

- Physically realistic predictions
- Prevents overfitting
- Better extrapolation
- Fewer training data points required → "Learning from physics"
- Better integration into Newton-type solvers like FEM

Choices for imposing physics-based constraints:

- Penalty methods
  - Special loss functions

Physics-constrained data-driven models

Imposing physics-based constraints has several advantages:

- Physically realistic predictions
- Prevents overfitting
- Better extrapolation
- Fewer training data points required → "Learning from physics"
- Better integration into Newton-type solvers like FEM

Choices for imposing physics-based constraints:

- Penalty methods
    - Special loss functions
- Exact methods

Physics-constrained data-driven models

Imposing physics-based constraints has several advantages:

- Physically realistic predictions
- Prevents overfitting
- Better extrapolation
- Fewer training data points required $\rightarrow$ "Learning from physics"
- Better integration into Newton-type solvers like FEM

Choices for imposing physics-based constraints:

- Penalty methods
  - Special loss functions
- Exact methods
  - Adherence to physics *everywhere*, not just on training region
  - *Guaranteed* results
  - Simpler loss function $\implies$ fewer computations
  - Better training due to simpler loss surface

Recent physics-informed data-driven models of hyperelasticity

Imposing physics-based constraints by design:

Recent physics-informed data-driven models of hyperelasticity

Imposing physics-based constraints by design:

- Constitutive Artificial Neural Networks (CANN)
- Input Convex Neural Networks (ICNN)
- Neural Ordinary Differential Equations (NODE)

Goals

Benchmark the models with experimental stress-stretch data

- Rubber $\rightarrow$ man-made material
    - Uniaxial Tension (UT)
    - Equibiaxial Tension (ET)
    - Pure Shear (PS)

Goals

Benchmark the models with experimental stress-stretch data

- Rubber $\rightarrow$ man-made material
  - Uniaxial Tension (UT)
  - Equibiaxial Tension (ET)
  - Pure Shear (PS)
- Skin $\rightarrow$ biological material
  - Strip biaxial X (SX)
  - Equibiaxial (EB)
  - Strip biaxial Y (SY)

Goals

Benchmark the models with experimental stress-stretch data

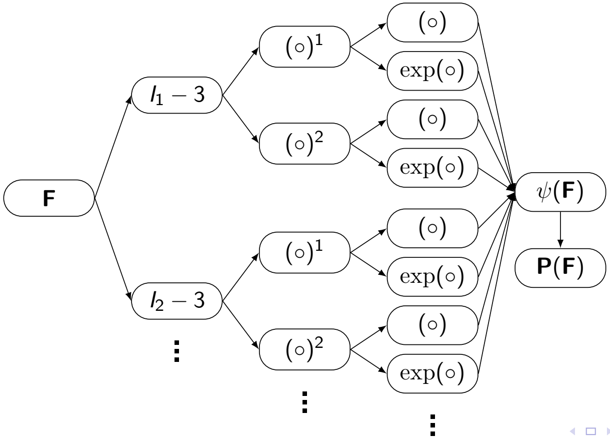
- Rubber $\rightarrow$ man-made material
  - Uniaxial Tension (UT)
  - Equibiaxial Tension (ET)
  - Pure Shear (PS)
- Skin $\rightarrow$ biological material
  - Strip biaxial X (SX)
  - Equibiaxial (EB)
  - Strip biaxial Y (SY)

Benchmarks considered:

- Training with rubber data
- Training with skin data
- Second derivatives of strain energy
- Model efficiency
- Extrapolation

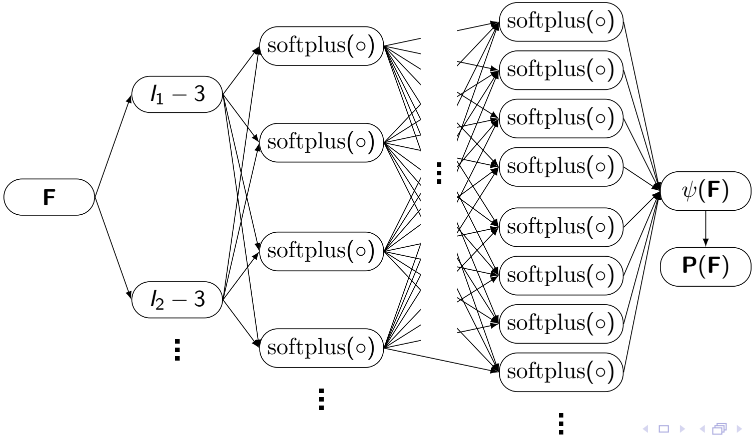
Constitutive Artificial Neural Networks (CANN)

- A century of work on constitutive material models
- Generalize widely used constitutive forms
- Reverse-engineer a strain energy function that is polyconvex by design
- Map $I_i(\mathbf{F}) \to \Psi(\mathbf{F})$ with CANNs and use $\Psi(\mathbf{F})$ to calculate the stress



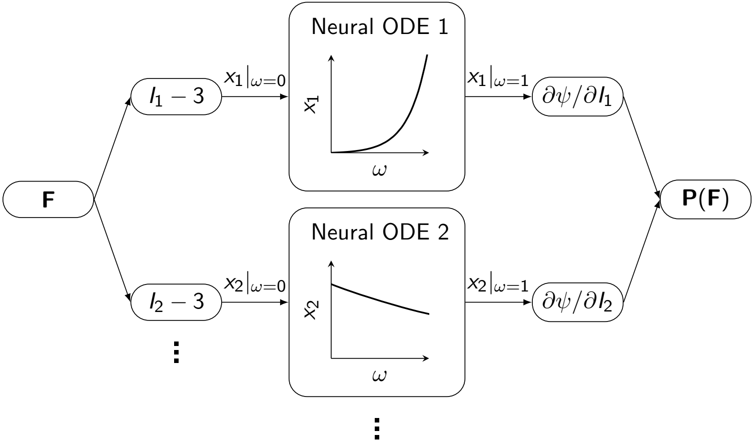
Input Convex Neural Networks (ICNN)

- $(f \circ g)(x)$ is convex if f is convex and g is convex and non-decreasing
- Use this with Feed Forward Neural Networks (FFNN)
- Use *softplus* activation functions with non-negative weights
- Map $I_i(\mathbf{F}) \rightarrow \Psi(\mathbf{F})$ with ICNNs and use $\Psi(\mathbf{F})$ to calculate the stress

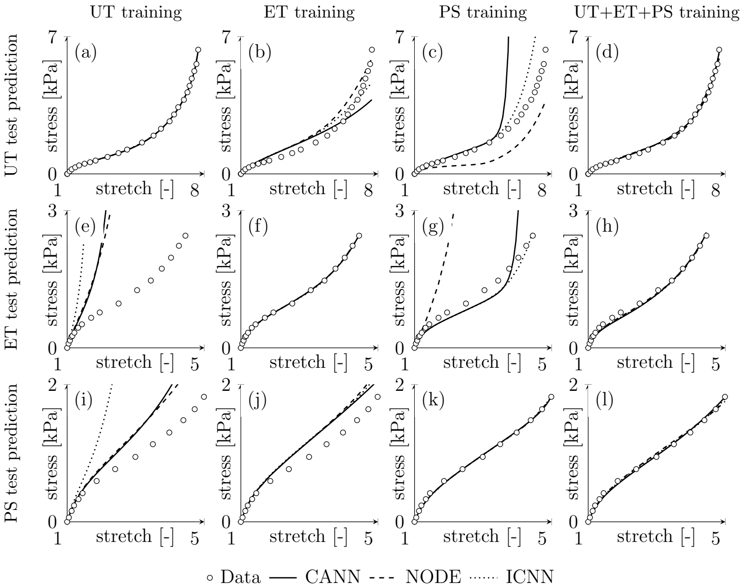


Neural Ordinary Differential Equations (NODE)

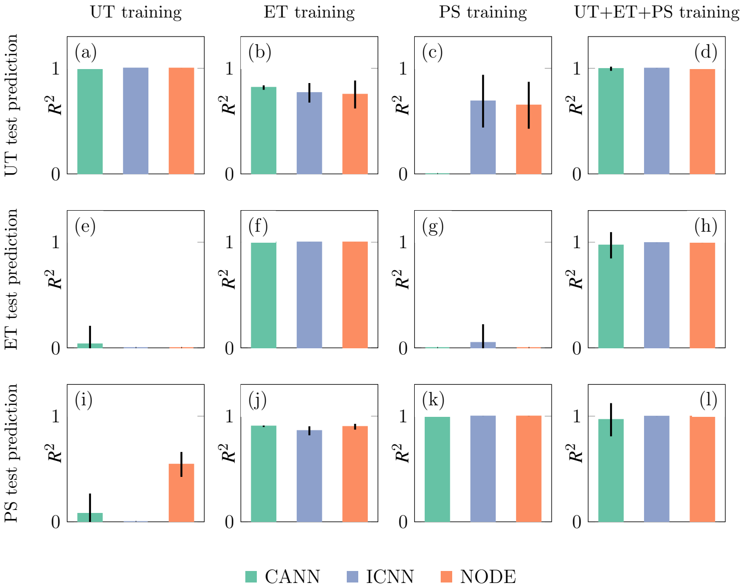
- NODEs are defined as the solutions of an ODE
- Solution trajectories of an ODE never intersect $\implies$ NODEs are monotonic operators
- $\partial f(x)/\partial x$ is monotonic $\iff$ $f(x)$ is convex
- Map $I_i(\mathbf{F}) \rightarrow \partial\Psi(\mathbf{F})/\partial I_i$ with NODEs and use $\partial\Psi(\mathbf{F})/\partial I_i$ to calculate the stress



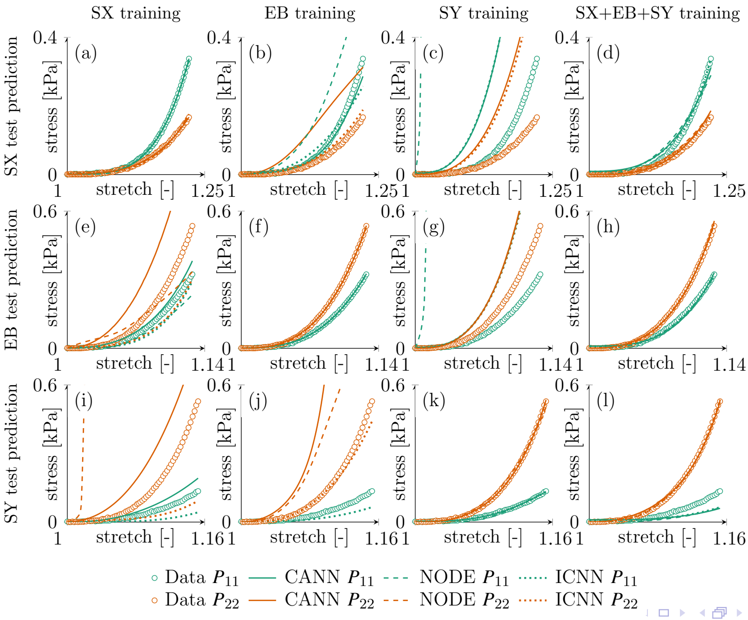
Training with rubber data



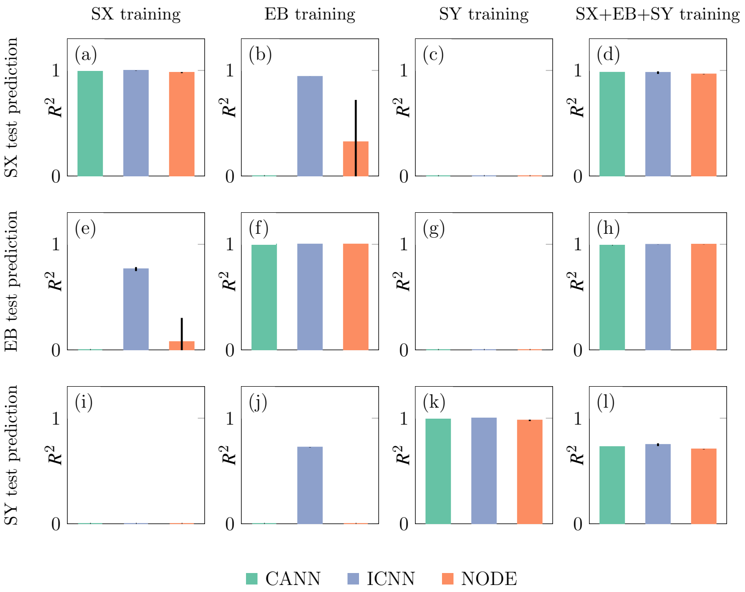
Training with rubber data



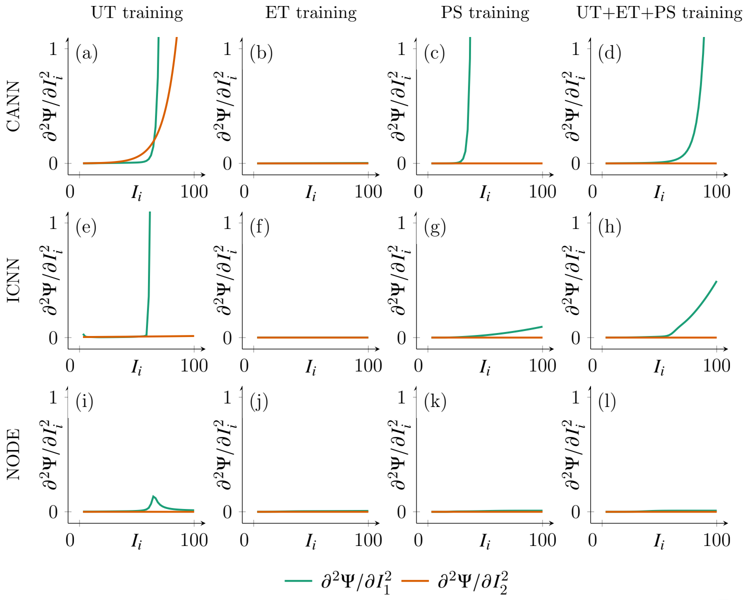
Training with porcine skin data



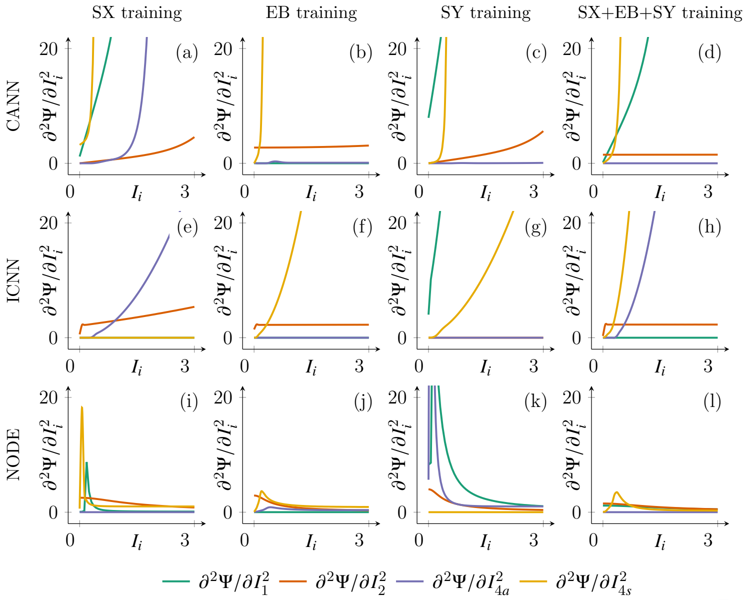
Training with porcine skin data



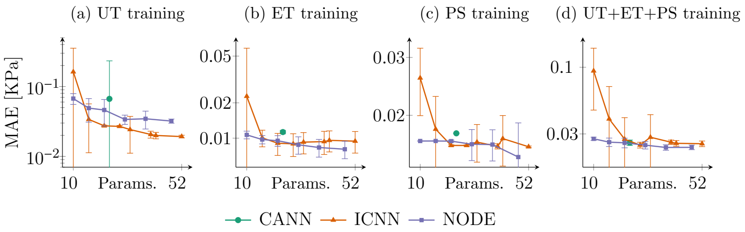
Second derivatives of strain energy (rubber)



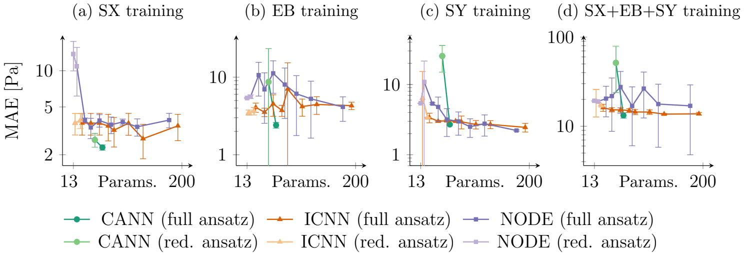
Second derivatives of strain energy (skin)



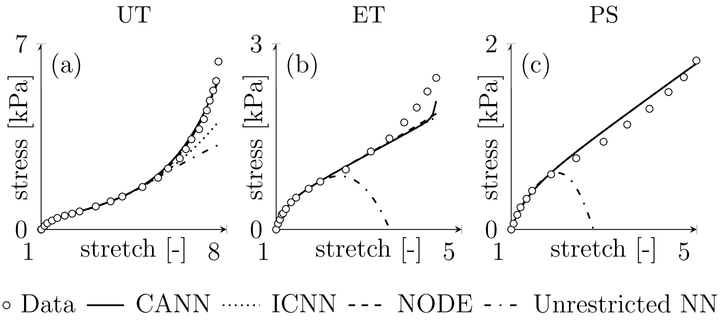
Model efficiency (rubber)



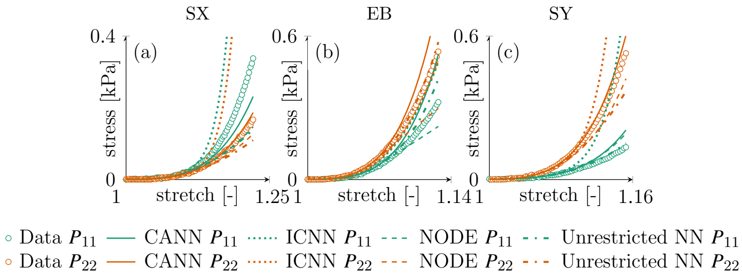
Model efficiency (skin)



Extrapolation (rubber)



Extrapolation (skin)



Conclusions

- All three models capture the training data almost perfectly
- Show some extrapolation capacity
- Second derivatives of strain energy are different
- The models show the expected trade-off in the number of parameters
- The methods are deemed sufficient to model the hyperelastic behavior of skin and rubber

Thank you!

V. Tac, K. Linka, F.S. Costabal, E. Kuhl, A. Buganza Tepole, "Benchmarks for physics-informed data-driven hyperelasticity", arXiv:2301.10714, 2023