Determining the Material Parameters of the Arterial Wall of a Mouse
– A comparison of computational approaches

A semester project in the LHTC

By

Bharath Narayanan

supervised by

Dr. Bram Trachet and Prof. Nikolaos Stergiopulos

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Motivation

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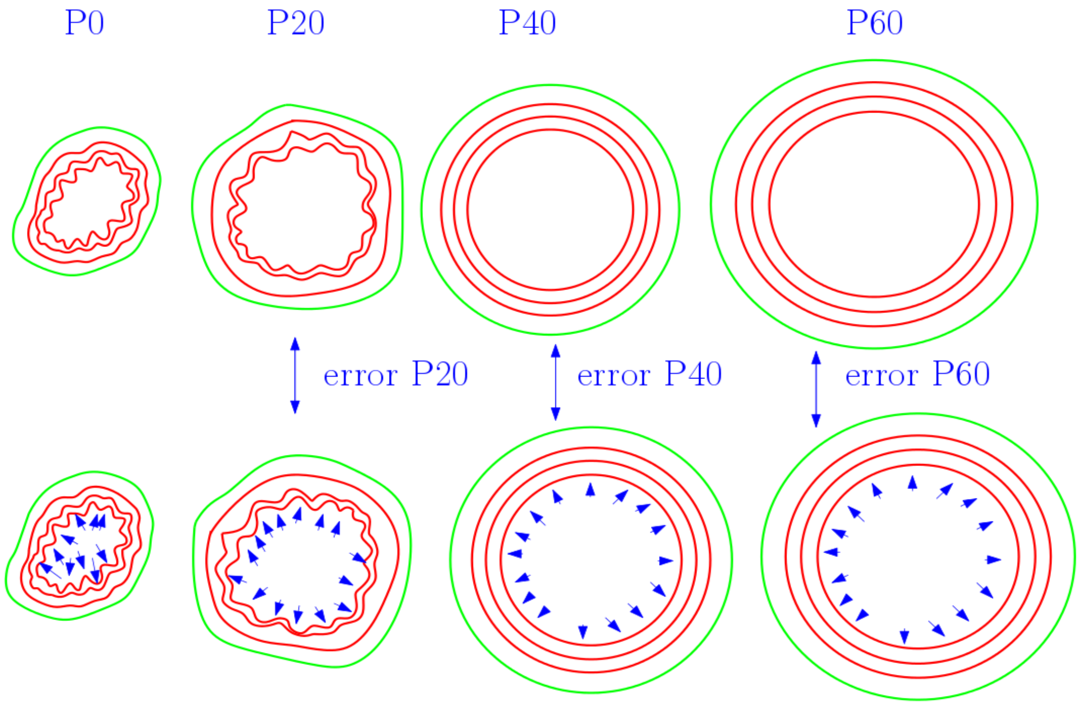
- The grand aim is to understand the link between aneurysims in mice and the mechanical properties of the lamellae.
- At the LHTC, we have microCTs of the aortic artery of a mouse at different pressure levels.
- Use finite element simulations and optimization algorithms to determine the material properties of the lamellar and interlamellar layers.



Objectives

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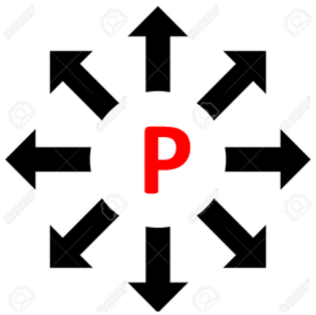
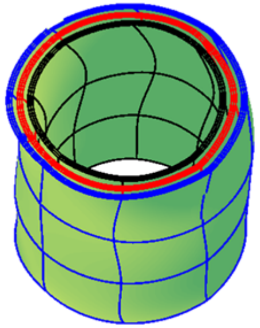
- Last semester : The validity of the tool chain (in the next slide) was established for a toy problem.
- The full problem is tackled this semester with an Arruda-Boyce material model.
- I compare three different methods for solving the optimization problem:
    - An Artificial Neural Network based surrogate model.
    - Direct finite differences (FD) using Matlab’s fmincon.
    - Semi-Analytical gradients (SA)

Tool Chain – Artery to NURBs curves

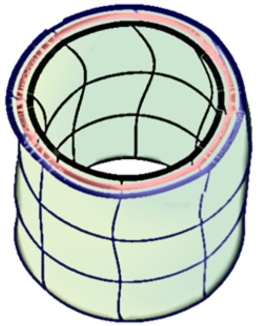


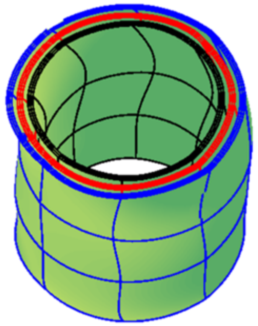


10 mm	CT_P10	Geom_P10
20 mm	CT_P20	Geom_P20
30 mm	CT_P30	Geom_P30
40 mm	CT_P40	Geom_P40
50 mm	CT_P50	Geom_P50
70 mm	CT_P70	Geom_P70
90 mm	CT_P90	Geom_P90
120 mm	CT_P120	Geom_P120

Tool Chain – NURBs curves to errors

Geom_P10





10 mm	Sim_P20	Geom_P20	E_1
20 mm	Sim_P30	Geom_P30	E_2
30 mm	Sim_P40	Geom_P40	E_3
40 mm	Sim_P50	Geom_P50	E_4
60 mm	Sim_P70	Geom_P70	E_5
80 mm	Sim_P90	Geom_P90	E_6
110 mm	Sim_P120	Geom_P120	E_7

FEAP Simulations

Setting up the Optimization Problem

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- Features:
  - Two materials - Lamellar and interlamellar layers.
  - Assumption – The materials follow the Arruda-Boyce hyper-elastic law.
  - Parameters per material :
    - Young’s modulus **Y**
    - Poisson’s ratio
    - *m* – A power law ratio

Parameter	**Lower Bound**	**Upper Bound**
Y (kPa)	50/180	400
ν	0.2	0.49
m	0.5	1.5

Setting up the Optimization Problem

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- We take an initial guess of material parameters **x.**
- We use the 10 mm Hg geometry as a base and apply the different pressures to it.
- We then calculate the 'error' at each pressure level: $$e_i = \sum_{j=1}^{N_{cp}} |\mathbf{r}_j^i - \hat{\mathbf{r}}_j^i|_{L2}$$
- The objective function to be minimized is the norm of this error vector: $$f(\mathbf{x}) = \sqrt{\sum_{i=1}^{7} e_i(\mathbf{x})^2}$$
- We use the gradients of the objective wrt **x** to determine the next choice of features that will bring us closer to the <u>minimum</u>.

$$\frac{df}{d\mathbf{x}} = \sum_{i=1}^{n} \frac{df}{de_i}\frac{de_i}{d\mathbf{x}}$$

Computational Approaches

- The objective function is determined in the same way regardless of the technique used.
- The differentiation comes when evaluating the gradients.

$$\frac{df}{d\mathbf{x}} = \sum_{i=1}^{n} \frac{df}{de_i} \frac{de_i}{d\mathbf{x}}$$

- Possible approaches:
  - **Artificial Neural Network** based surrogate model.
  - **Finite Difference Gradients**
  - **Semi-Analytical Gradients**

ARTIFICIAL NEURAL NETWORK BASED SURROGATE MODEL

Create a <u>surrogate model</u> using artificial neural networks and then optimize using this surrogate model.

https://hackernoon.com/convolutional-neural-network-in-5-minutes-8f867eb9ca39

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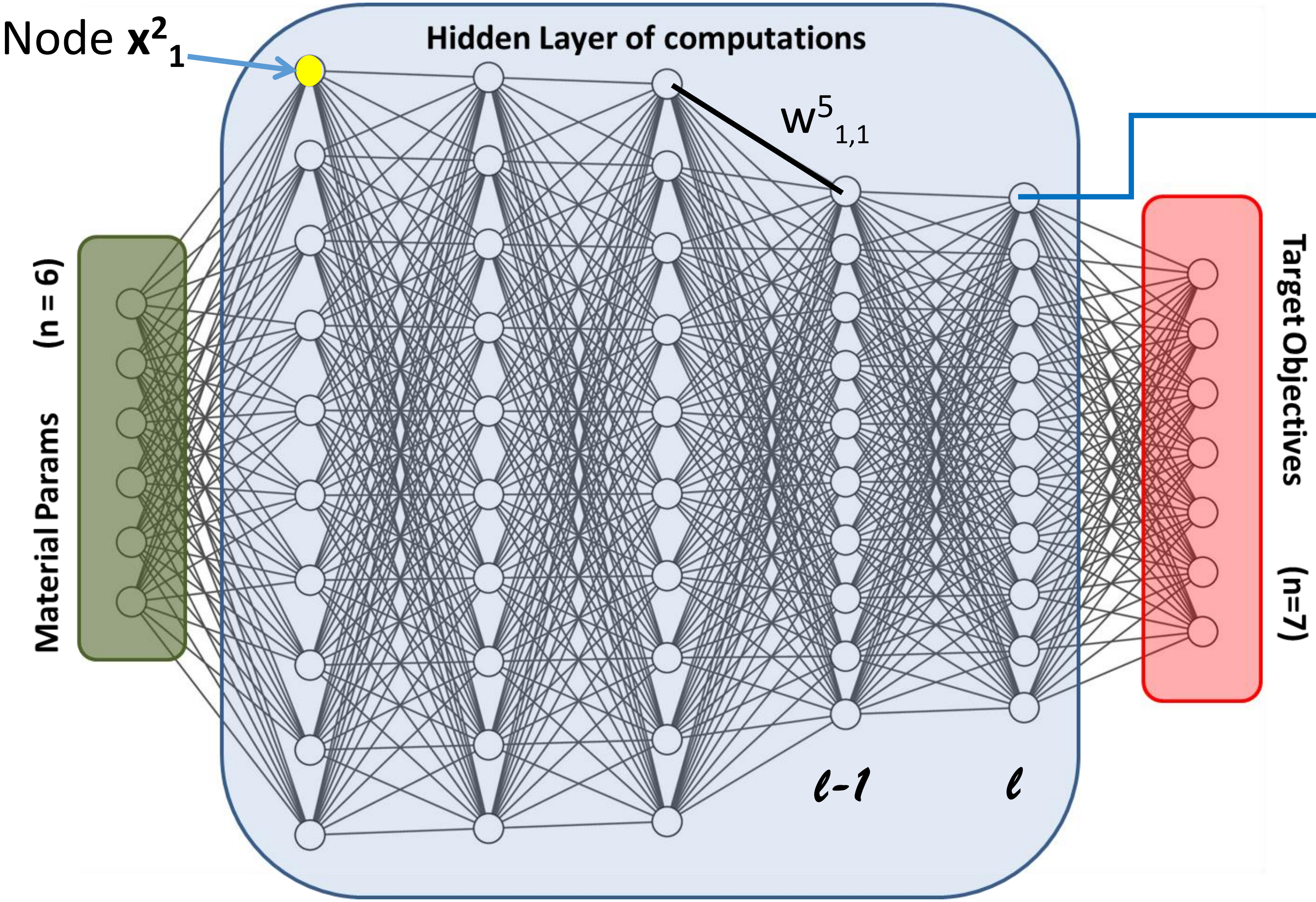
What are Artificial Neural Networks?



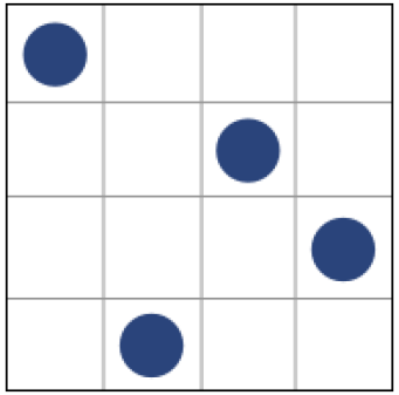
$$z_j^l = \sum_{i=1}^{N} w_{i,j}^l x_i^{l-1}$$

$$x_j^l = \phi(z_j^l)$$

Activation function

Creating our Surrogate Model

- 500 simulations within the design space.
- Design space specified using bounds shown earlier.
- We use Latin-HyperCube sampling to ensure that the space is well filled.
- We then have **500 samples** of data, each having 6 inputs and 7 outputs.
- We use **450** out of 500 samples to ***train*** the network with various parameters.
- The remaining **50** are used to ***test*** the network's predictive capabilities.



Metric	Value (%)
Mean Error	0.236 ± 0.215
Maximum Error	6.050 ± 9.121
Median Error	0.057 ± 0.024

Final ANN Surrogate Model

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Hyperparameter	Value	Space
Optimizer	Adam	Adam, SGD, Adamax
Learning Rate	0.001	0.0001 .. 0.1
Hidden layers	2	2
Neurons per layer	50 (layer 1), 30 (layer 2)	5 .. 40,50 (each layer)
Activation function	sigmoid	sigmoid, tanh, relu
Epochs	1500	1500, 2000
Batch Size	10	10 .. 100

Once the surrogate model is obtained, the analytical gradients of the output wrt the input are automatically available!!

GRADIENTS USING FINITE DIFFERENCES

Finite Difference Gradients

- Simplest to implement.
- At each point in the design space, **6** more simulations are conducted in order to determine the gradient using forward finite differences.
- Each simulation takes **~4 minutes**.

VERY EXPENSIVE!!!

SEMI-ANALYTICAL GRADIENTS

Semi-Analytical Gradients

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- The finite difference approach needs 7 simulations at each point in feature space.
- In order to reduce the computational cost, I use the tangent stiffness matrix **K** and the residual vector **f** from the FEAP simulations themselves to obtain the semi-analytical gradients.
- This method only requires 1 simulation at each point, combined with vector assembly which takes only a few seconds. In addition, it needs some <u>sparse matrix algebra</u>.

Semi-Analytical Gradients

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- Each simulation solves a nonlinear system of equations defined by :

$$f(\mathbf{x}, \mathbf{u}) = 0$$

Where ***f*** is the residual vector.

- The total derivative of the nonlinear system wrt the material parameters should be 0.

$$\frac{D\mathbf{f}}{D\mathbf{x}} = 0 \qquad \boxed{\Longrightarrow \frac{df}{d\mathbf{x}} + \frac{df}{d\mathbf{u}}\frac{d\mathbf{u}}{d\mathbf{x}} = 0}$$

- Finally, we obtain the derivative of the errors at each pressure level wrt the material parameters:

$$\frac{de_i}{d\mathbf{x}} = \frac{de_i}{d\mathbf{u}}\frac{d\mathbf{u}}{d\mathbf{x}} \qquad \Longrightarrow \qquad \boxed{\frac{de_i}{d\mathbf{x}} = -\frac{de_i}{d\mathbf{u}}\left(\frac{df}{d\mathbf{u}}\right)^{-1}\frac{df}{d\mathbf{x}}}$$

- Determine using FD
- Only requires vector assembly
- **INEXPENSIVE!!!!!**

Tangent stiffness matrix

RESULTS

ANN Surrogate Model

- Generating the data took around **5 hours.** The optimization on the surrogate model was done using **SQP.**
- In order to determine the veracity of the entire ANN model, we took the optimum feature set predicted by the ANN and ran a simulation with it. We then compared the predicted and actual simulation error at each pressure level.

OPTIMIZATION RESULT

Output	E-1	E-2	E-3	E-4	E-5	E-6	E-7
Sim.	12.51	13.47	19.05	19.45	19.48	23.25	27.10
Optim.	12.50	13.47	19.08	19.46	19.43	23.18	27.41
% Diff.	0.07	0.008	0.2	0.07	0.27	0.3	1.13

Optimum obj. fn. value: 52.41 (predicted) 52.28 (simulated)

ANN Surrogate Model - Robustness

COMPARISON OF 3 DIFFERENT RUNS - PROPERTIES OF LAMELLAR AND INTER-LAMELLAR LAYERS

Output	Lamellar			Inter-Lamellar		
	Y (kPa)	ν	m	Y(kPa)	ν	m
Run-1	50	0.2	0.74	330	0.44	1.5
Run-2	50	0.38	0.984	394	0.297	1.5
Run-3	50	0.49	0.872	306	0.45	1.5

COMPARISON OF 3 DIFFERENT RUNS - OUTPUTS OF FUNCTION MINIMA

Output	E-1	E-2	E-3	E-4	E-5	E-6	E-7
Run-1	12.50	13.47	19.08	19.46	19.43	23.18	27.41
Run-2	12.52	13.55	19.34	19.78	19.85	23.46	27.90
Run-3	12.29	13.27	18.78	19.27	19.51	23.29	27.30

Finite-Difference Based Gradients

FUNCTIONAL EVALUATIONS USING FINITE-DIFFERENCE GRADIENTS.

Iter	F-count	f(x)	Optimality	Step-size	Time (s)
0	7	58.869	1.48E+08		1992.857312
1	16	55.230	2.61E+07	5.54E-03	4016.841834
2	23	53.592	1.69E+07	7.93E-01	5495.904916
3	31	52.882	2.46E+07	1.26E-01	7318.828766
4	**39**	**52.174**	**4.64E+06**	**5.93E-02**	**9250.484152**
5	47	51.996	2.72E+07	2.37E-02	11138.59503
6	54	51.946	2.16E+06	1.27E-01	12776.42802
7	61	51.840	7.48E+05	5.32E-02	14421.50157
8	68	51.780	5.74E+06	4.18E-02	16039.20439
9	75	51.788	2.47E+06	9.78E-03	17711.38578
10	82	51.773	1.55E+06	1.70E-02	19391.56054

Obj fn lower than ANN.

Semi-Analytical Gradients

FUNCTIONAL EVALUATIONS USING SEMI-ANALYTICAL GRADIENTS.

Iter	F-count	f(x)	Optimality	Step-Size	Time (s)
0	1	58.869	1.49E+08		467.94434
1	4	55.230	2.49E+07	5.47E-03	1922.789478
2	5	53.626	1.62E+07	7.78E-01	2436.565702
3	7	52.947	2.75E+07	1.37E-01	3476.453458
4	9	52.859	5.40E+07	4.54E-02	4521.581669
5	**10**	**52.094**	**3.76E+07**	**1.38E-01**	**5041.03577**
6	12	52.001	8.74E+06	8.35E-02	6141.814817
7	14	51.918	3.03E+07	8.61E-02	7190.015427
8	15	51.836	5.16E+06	1.07E-01	7721.143276
9	16	51.806	5.63E+05	4.56E-02	8249.961671
10	17	51.778	1.82E+06	4.07E-02	8775.145602

Obj fn lower than ANN.

Feature Vector Comparison

COMPARISON OF METHODS - PROPERTIES OF LAMELLAR AND INTER-LAMELLAR LAYERS.

Method	**Lamellar**			**Inter-Lamellar**		
	Y (kPa)	ν	**m**	**Y(kPa)**	ν	**m**
ANN	50	0.2-0.49	0.74 - 0.984	306-394	0.3 - 0.45	1.5
FD	89.7	0.46	1.28	238	0.474	1.38
SA	90.67	0.452	1.26	238.25	0.475	1.382
Literature	46-113	0.4	0.98	136-350	0.4	0.98

A. Danpinid, J. Luo, J. Vappou, P. Terdtoon, and E. E. Konofagou, "In vivo characterization of the aortic wall stress–strain relationship," *Ultrasonics*, vol. 50, no. 7, pp. 654–665, 2010.

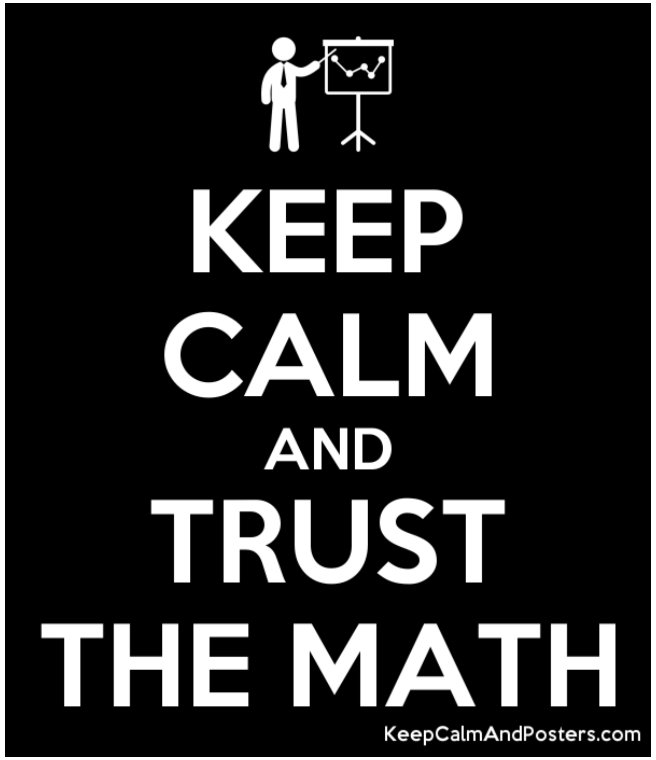
CONCLUSION

Overview of Techniques

- **ANN:**
  + **Versatile - can be used for extremely nonlinear problems**
  + **Scales well – parallelization possible!**
  - **Cannot predict outside the bounds provided.**
  - **Needs tuning which might change with each new dataset.**
- **Finite Difference**
  + **Robust**
  + **Versatile – only the step size for the FD gets smaller for nonlinear problems.**
  - **Does not scale well with more parameters or finer mesh sizes.**
- **Semi-Analytical**
  + **Robust, mathematically sound.**
  + **Efficient with time and scales well with more parameters and finer mesh sizes.**
  - **For extremely non-linear problems, the semi-analytical gradients may not be accurate.**

Final Verdict

- Considering scalability and robustness, the Semi-Analytical gradient method is suitable for the problem at hand.
- ANN surrogate models can be extremely useful in the case of very complex material models and larger design spaces.
- However, one must be very careful to ensure that the predictions of the neural network are reliable and consistent. This requires a lot of time in testing and validation.
- The semi-analytical gradient method can be verified mathematically. Once it is validated for a problem, the system remains the same regardless of scale or complexity.



https://www.keepcalmandposters.com/poster/5841664_keep_calm_and_trust_the_math

Future Work

- Include adventitia in geometry modelling.
- Refine the mesh further.
- Treat each layer as a separate material.
- Introduce spatially varying thickness of the lamellar layers.
- Use a more complex non-linear material model for the interlamellar layers.