Implementing integrated machine learning strategies to accelerate high accuracy fracture growth simulators

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Agenda

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- Background: SIF
- Problem Specification
- Implementation
- Testing Strategy
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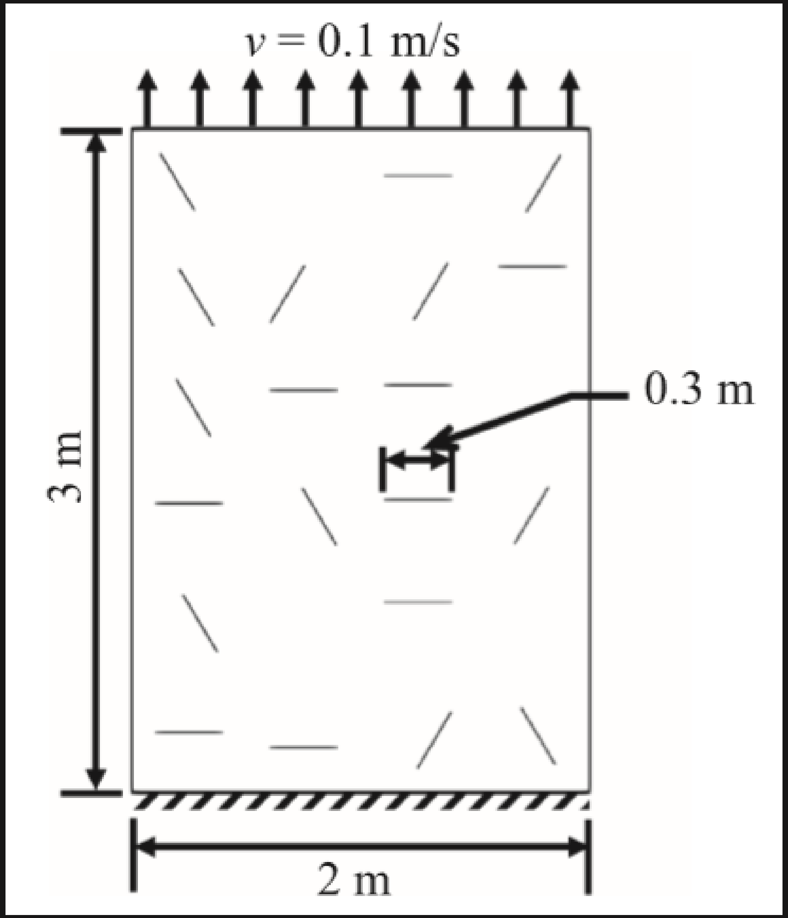
Motivation

- Fracture Simulation is of great importance to many fields
  - Hydraulic Fracturing
  - Mineral Extraction
  - Medical Osteology
- FDEMs are very accurate but can be slow
- Is it possible to improve time efficiency without loss of accuracy?

Introduction

- ML has been applied to fracture problems before
- Can be effective for certain criteria
- Often limited by:
  - Restricted dimensionality
  - Graph theoretic approach
- Not currently applicable to real world problems



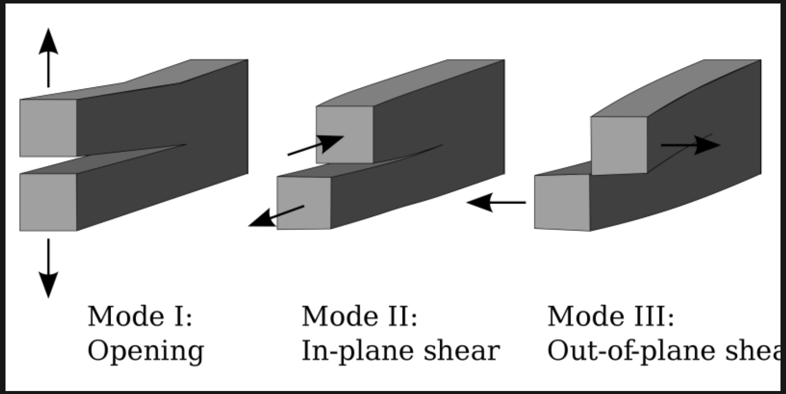
Source: (Hunter, et al., 2019)

Introduction

- Avoid aforementioned limitations by accelerating an FDEM
- Calculation of SIF required before fracture tip evolution
- SIF computation requires solution of several PDEs – computationally complex
- Fracture tip evolution is well understood and simple by comparison
- Is it possible to predict the SIF without the preceding computation?

Background: SIF

- Most important quantity for this project is Stress Intensity Factor (SIF)
- The SIF is a theoretical construct that encodes the stress state at a tip
- SIF has three elements:
  - K_I - opening damage – positive definite
  - K_{II} - in-plane shearing
  - K_{III} - out-of-plane shearing



- K_I is often dominant, K_{II} and K_{III} are harder to predict

Problem Specification

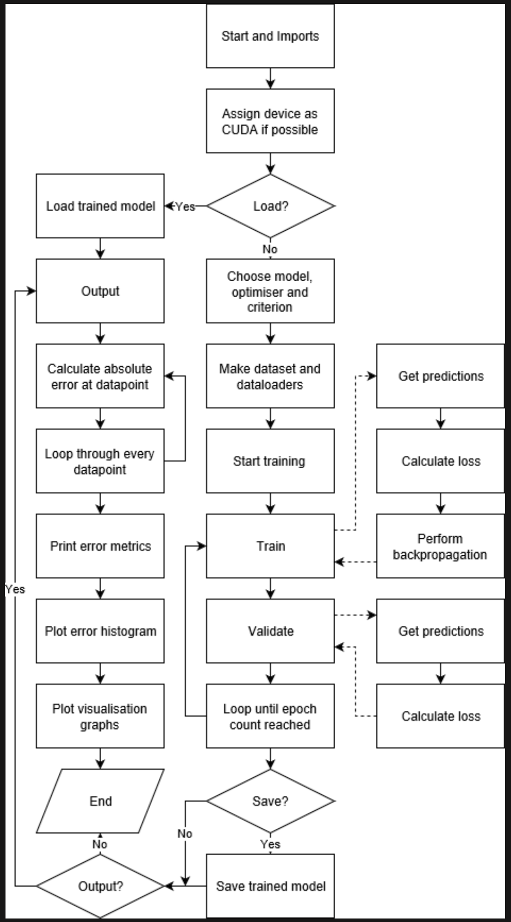
- Two factors relevant to an accelerator:
  - Time efficiency
  - Accuracy
- For an ML method, time efficiency applies to training and execution
  - Training time of diminished importance
  - Execution time almost guaranteed to be superior to current algorithm
- Therefore primary objective is accuracy retention

Problem Specification

- This is a regression problem
- Fracture tip evolution is determined by the current configuration
  - Therefore configuration history information is not necessary
- Inter-fracture geometric data is important for interactions
- Data is gathered from runs of the Imperial College Geomechanics Toolkit (ICGT)

Implementation

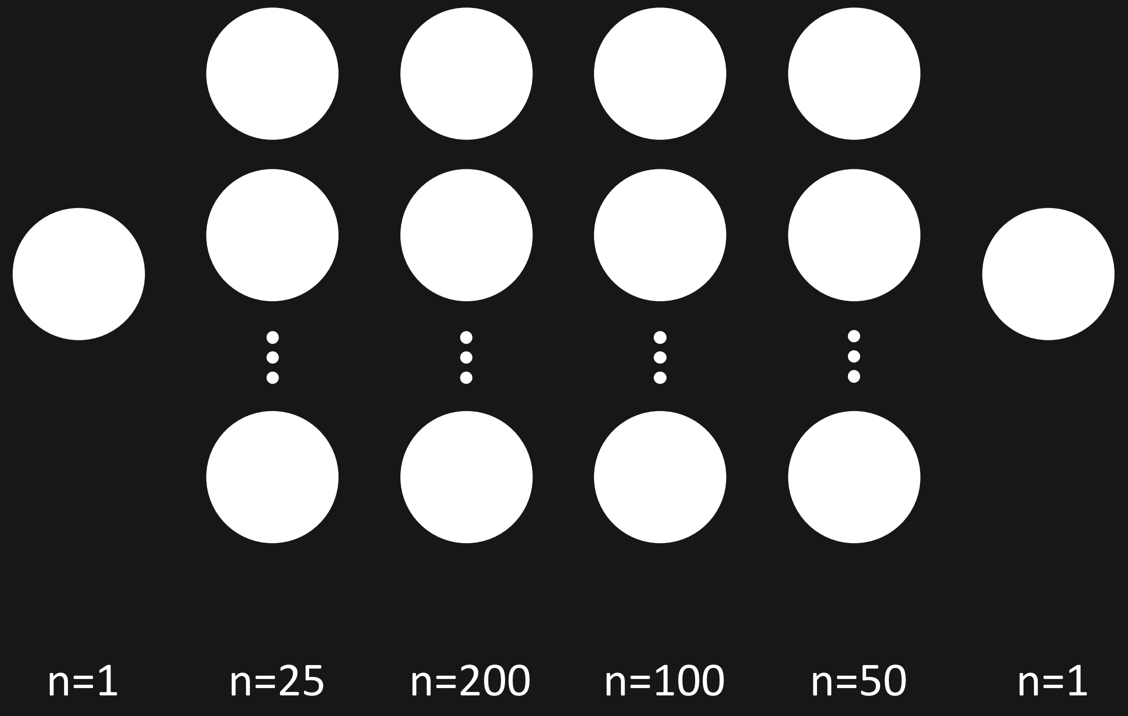
- Feed forward neural network selected
- Python implementation – chosen for ML libraries
- PyTorch used for the ML aspects
- Little attention given to hyperparameters at this stage
- Input data formatted as a CSV
- Data split as 80:10:10 for training : validation : testing



Testing Strategy

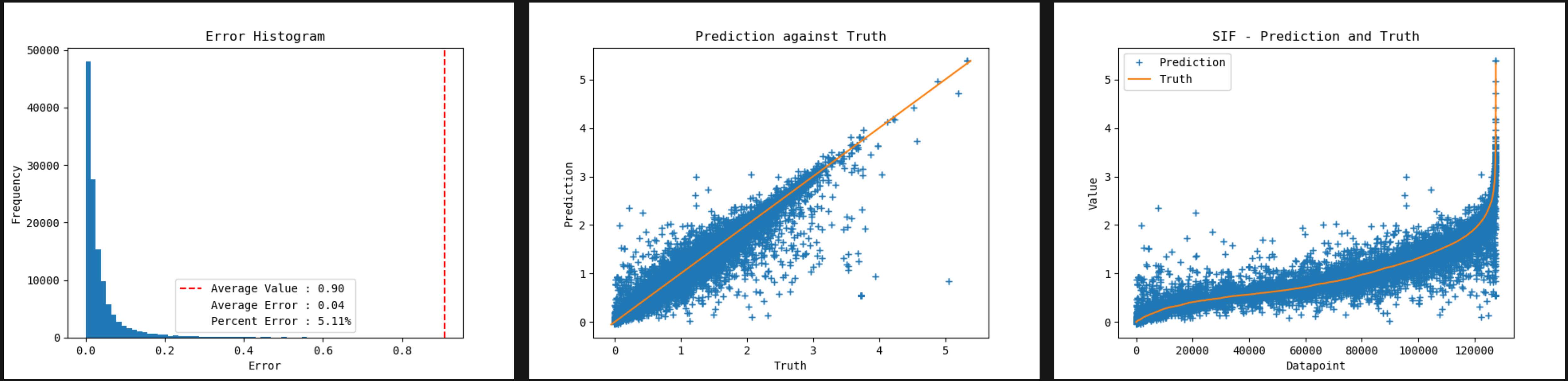
- Testing strategy designed for hyperparameter optimisation
- Optimal configuration infeasible to ascertain
- Heuristic approach taken
  - Hyperparameters tested in order of expected significance
  - Order investigated with preliminary testing
- Will not result in optimal configuration, but adequate
- Hyperparameters tested are:
  - Feature set
  - Model architecture
  - Optimiser
  - Criterion function
  - Activation function
- Further hyperparameters left as defaults

Testing Conclusions



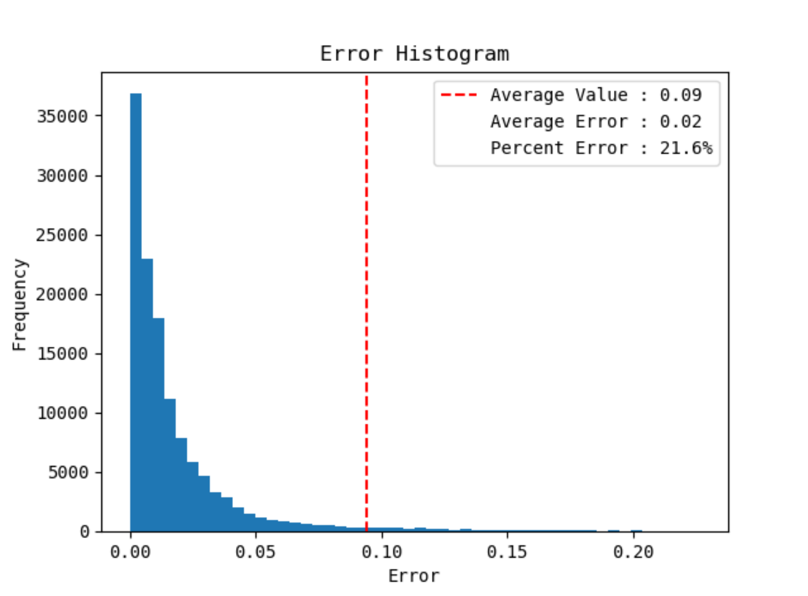
- Feature Set: position vector, orientation vector, old SIF
- Architecture: see diagram
- Optimiser: Adam
- Criterion Function: L1Loss
- Activation Function: LeakyReLU

Results - K_I

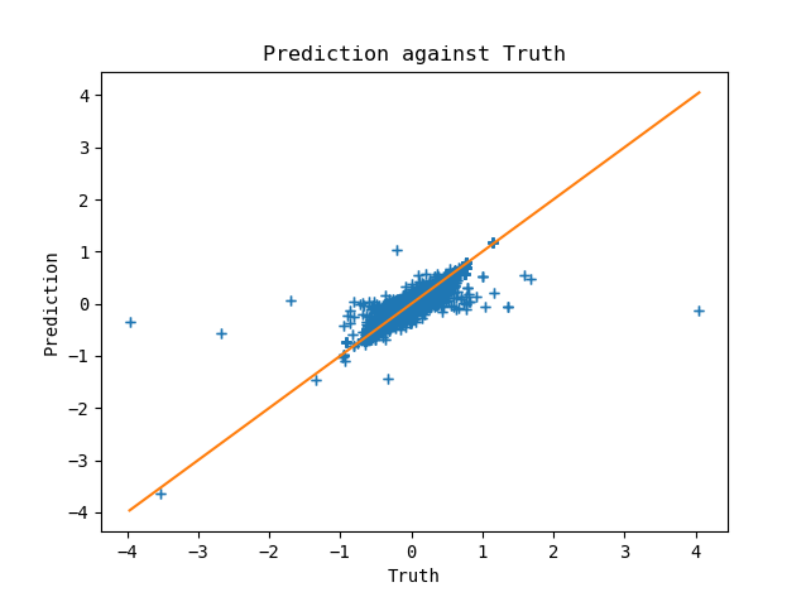


Error Histogram
Frequency
Error
Average Value : 0.90
Average Error : 0.04
Percent Error : 5.11%
Prediction against Truth
Prediction
Truth
SIF - Prediction and Truth
Prediction
Truth
Value
Datapoint

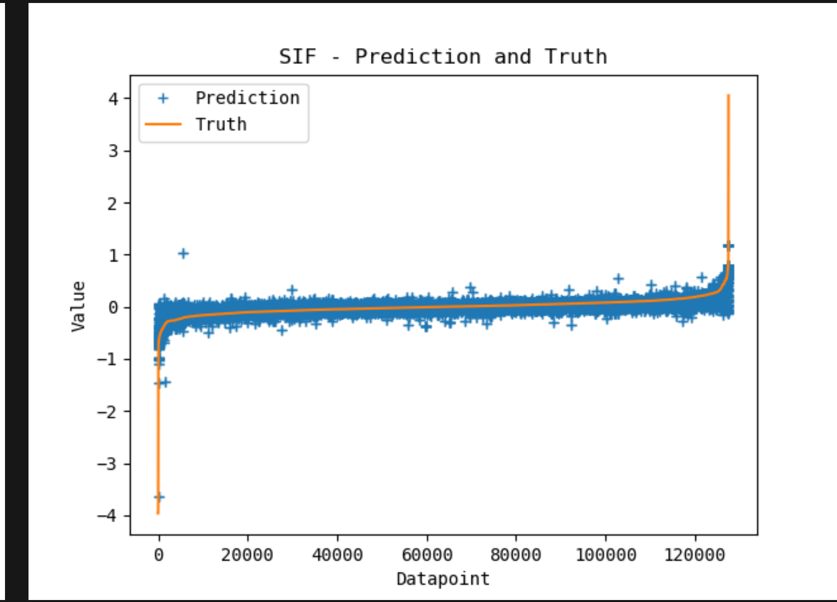
Results - K_{II}



Error Histogram
Average Value : 0.09
Average Error : 0.02
Percent Error : 21.6%
Frequency
Error
35000
30000
25000
20000
15000
10000
5000
0
0.00
0.05
0.10
0.15
0.20

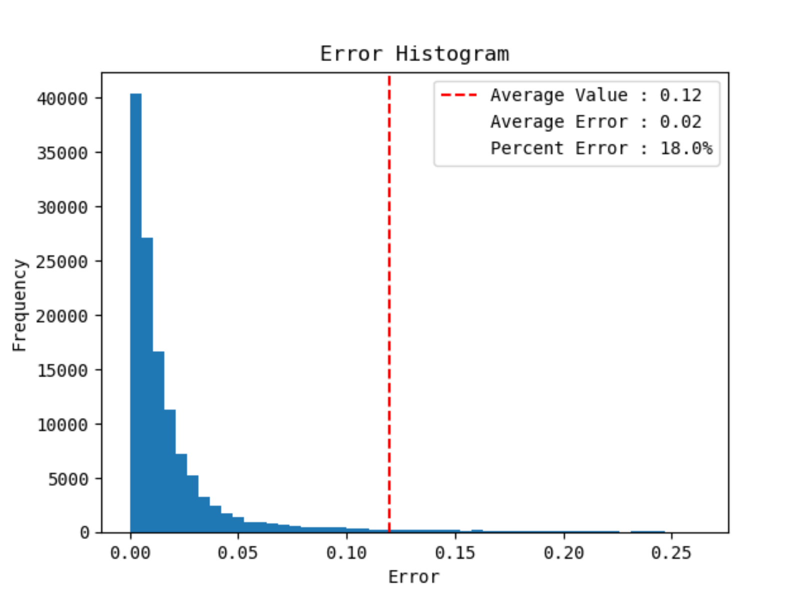


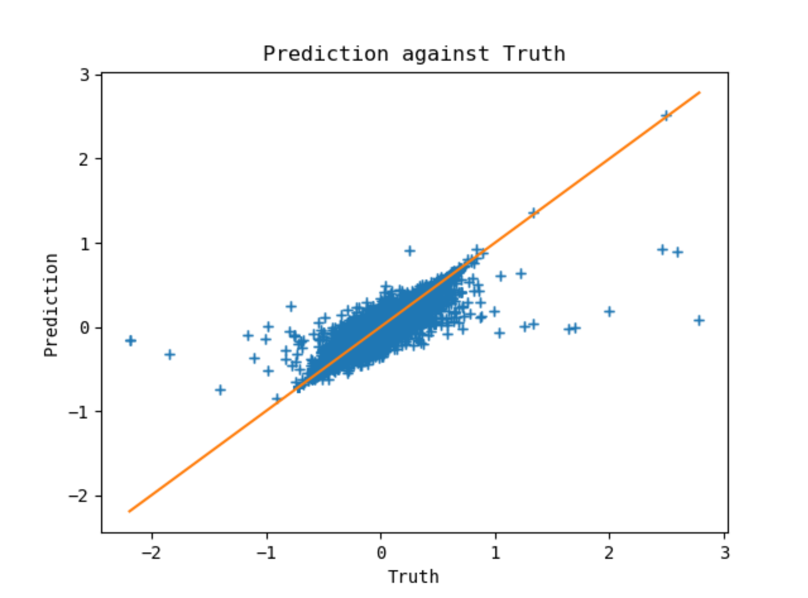
Prediction against Truth
Prediction
Truth
4
3
2
1
0
−1
−2
−3
−4

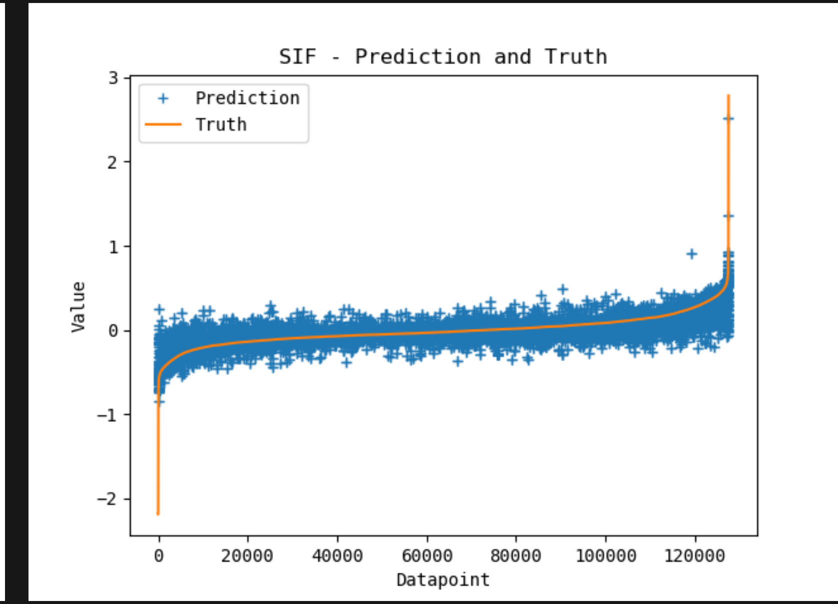


SIF - Prediction and Truth
Prediction
Truth
Value
Datapoint
0
20000
40000
60000
80000
100000
120000

Results - K_{III}





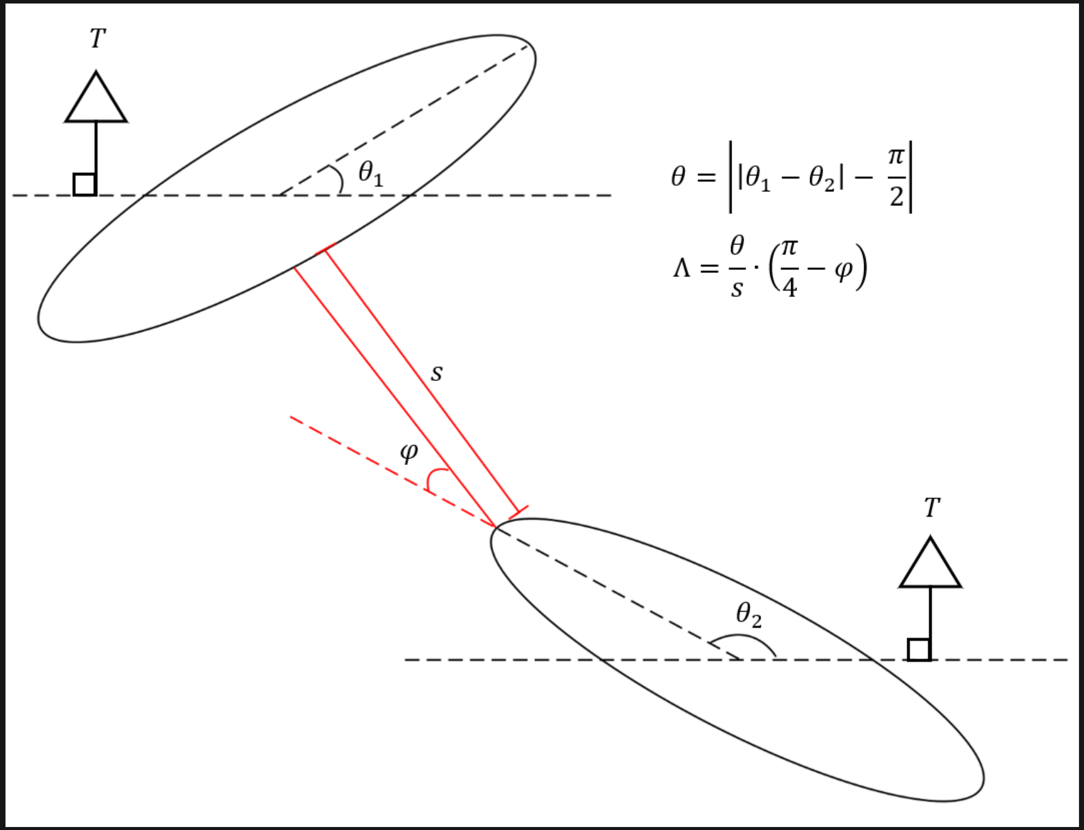


Conclusions

- ML acceleration of an FDEM is viable
- K_I easier to predict than K_{II} and K_{III}
- Further inter-fracture geometric data must be incorporated into feature set
- Outputs currently returned with insufficient accuracy for immediate practical implementation

Future Developments

- Increased dataset size
- Improved hyperparameter optimisation scheme
- Addition of fracture interaction index – see diagram
- Implementation of binary measure for fracture interaction



Thank you for your attention

Any questions?