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Sandia National Laboratories

Elastic Model Calibration using Dakota

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Outline

Introduction

Functional Data Analysis

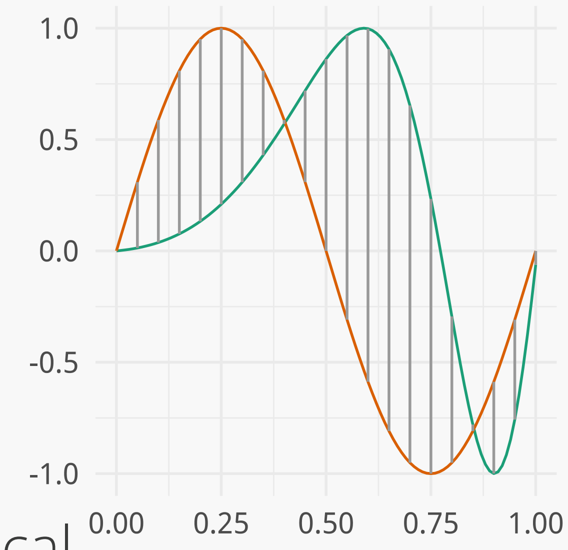
- Elastic Metric

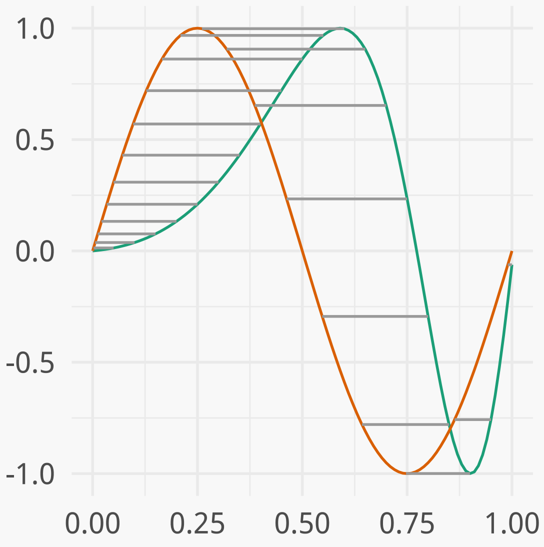
Model Calibration using Dakota

Results

Introduction

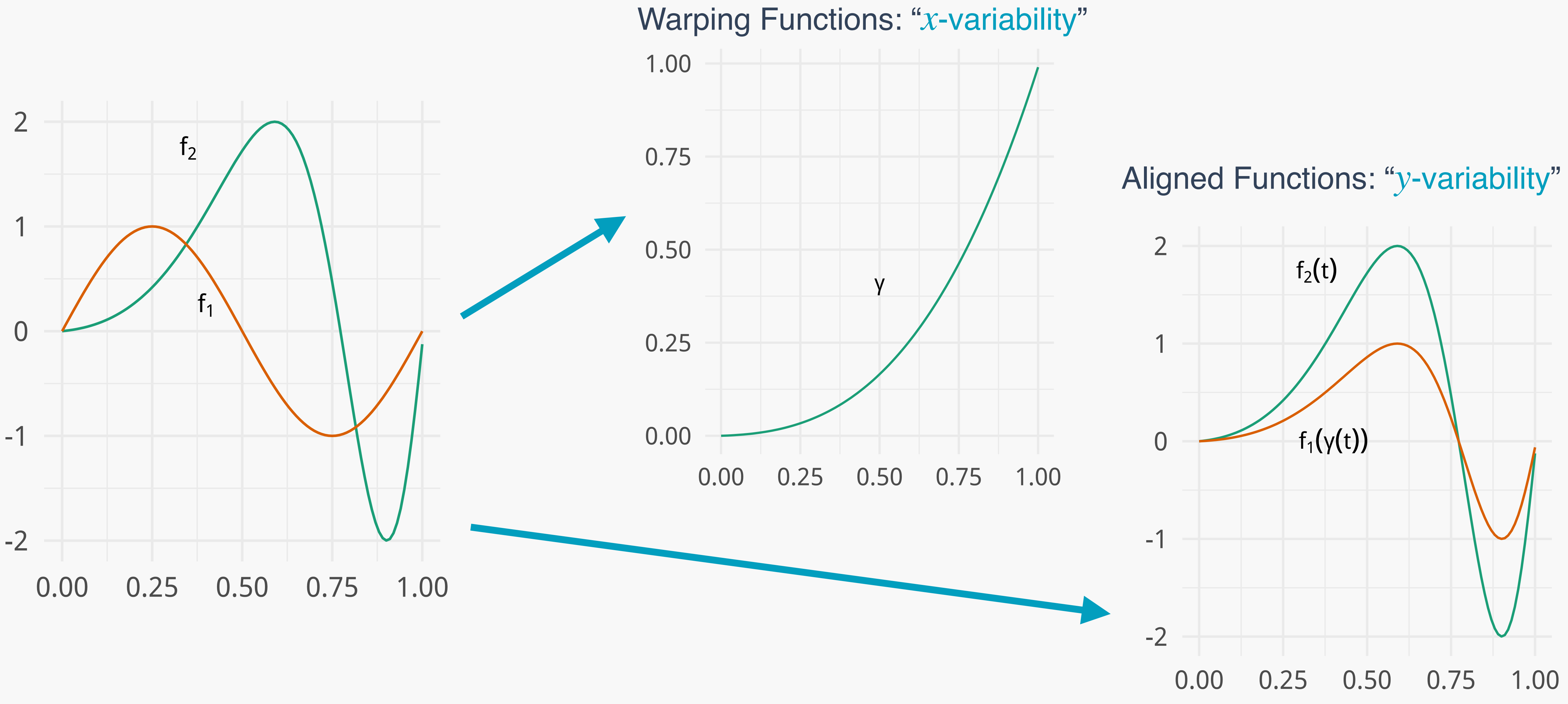
- Question arise on how can we model functions
  - Can we use the functions to classify diseases?
  - Can we use them as predictors in a regression model?
  - Can we calibrate a computer model?
- It is the same goal (question) of any area of statistical study





- One problem occurs when performing these type of analyses is that functional data can contain variability in time (x-direction) and amplitude (y-direction)
- How do we account for and handle this variability in the models that are constructed from functional data?

Components of Function Variability



Functional Data Analysis

Let f be a real valued-function with the domain $[0,1]$, can be extended to any domain

- Only functions that are absolutely continuous on $[0,1]$ will be considered

Let Γ be the group of all warping functions

$$\Gamma = \{\gamma : [0,1] \rightarrow [0,1] \,|\, \gamma(0) = 0, \gamma(1) = 1, \ \gamma \text{ is a diffeo}\}$$

It acts on the function space by composition

$$(f, \gamma) = f \circ \gamma$$

It is common to use the following objective function for alignment

$$\min_{\gamma \in \Gamma} \|f_1 \circ \gamma - f_2\|$$

Note: It is not a distance function since it is not symmetric.

Elastic Distance (Fisher-Rao)

Define the Square Root Velocity Function

$$q : [0,1] \to \mathbb{R}^1,\ q(t) = sign(\dot{f}(t))\sqrt{|\dot{f}(t)|}$$

Fisher Rao Distance is $\mathbb{L}^2$ in SRVF space

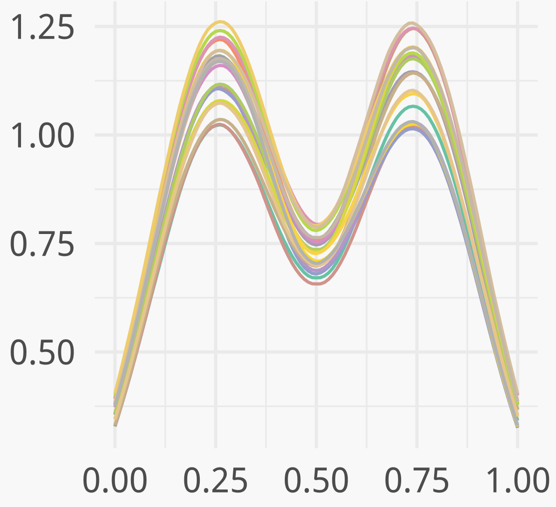
$$d_a(f_1, f_2) = \inf_{\gamma} \|(q_1 \circ \gamma)\sqrt{\dot{\gamma}} - q_2\|$$

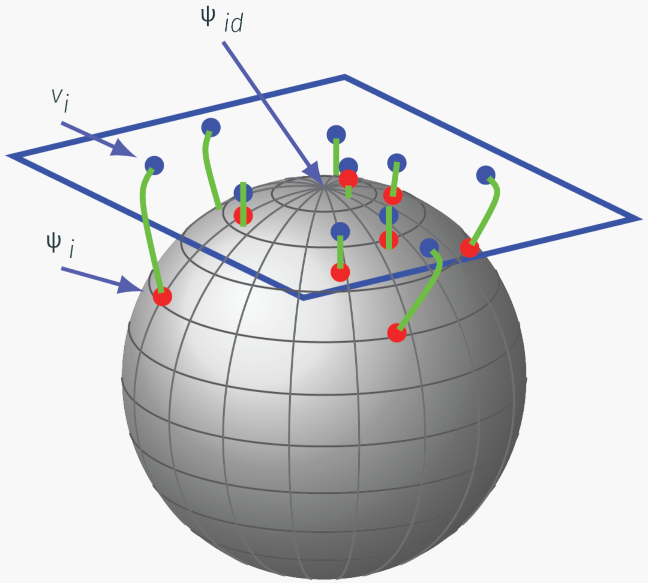
Distance is a proper distance

- symmetric, isometric, triangle inequality

Can compute distance on warping functions (how much alignment)

$$d_p(\gamma) = \arccos\left(\int_0^1 \sqrt{\dot{\gamma}}\, dt\right)$$





Calibration Framework

Given a computational model, M with parameters θ

We wish to find an optimal θ^* such that the computation prediction $f(\theta)$ matches the experimental data f_E

The optimal θ^* is found by either minimizing the following three cases:

$$\arg\min_{\theta} d_a(f_E, f(\theta))$$ Amplitude Only

$$\arg\min_{\theta} d_p(\gamma(\theta))$$ Phase Only

$$\arg\min_{\theta} \tau d_a(f_E, f(\theta)) + (1-\tau) d_p(\gamma(\theta)$$ Balance Amplitude and Phase

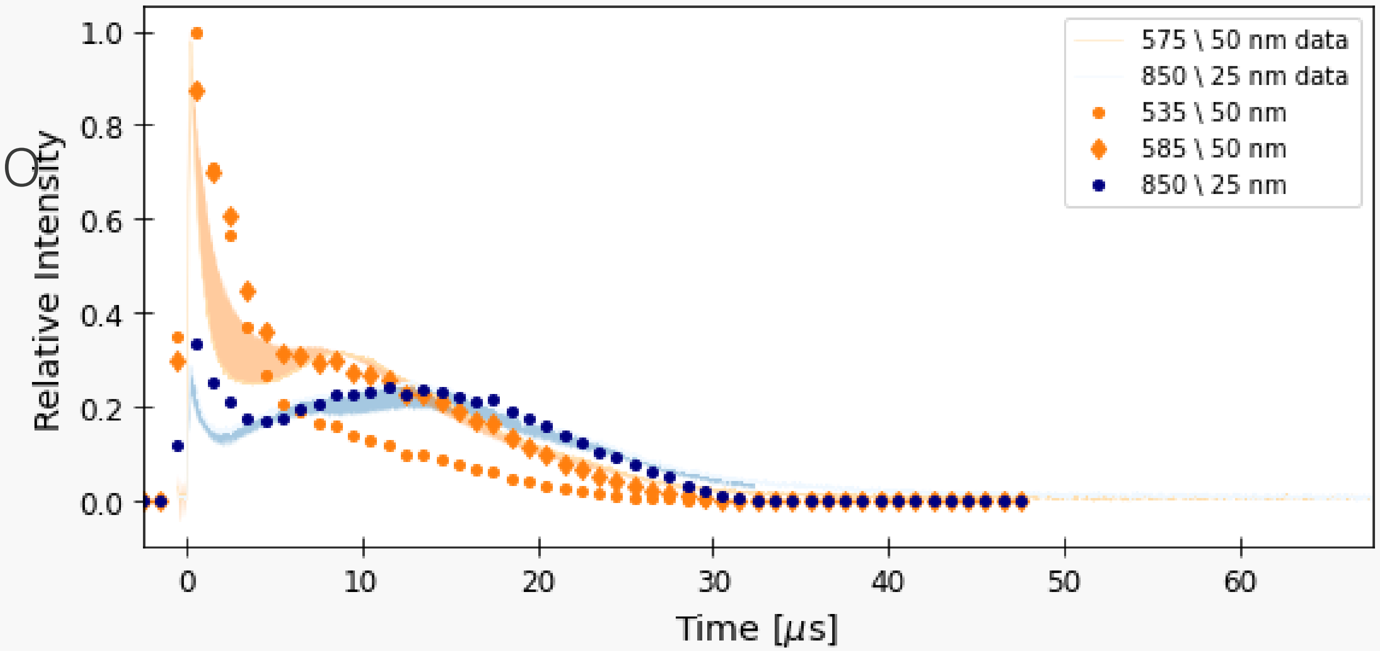
Results

Performed optimization using Dakota framework

- Utilized python extension to talk to elastic FDA python package (`fdasrsf`)

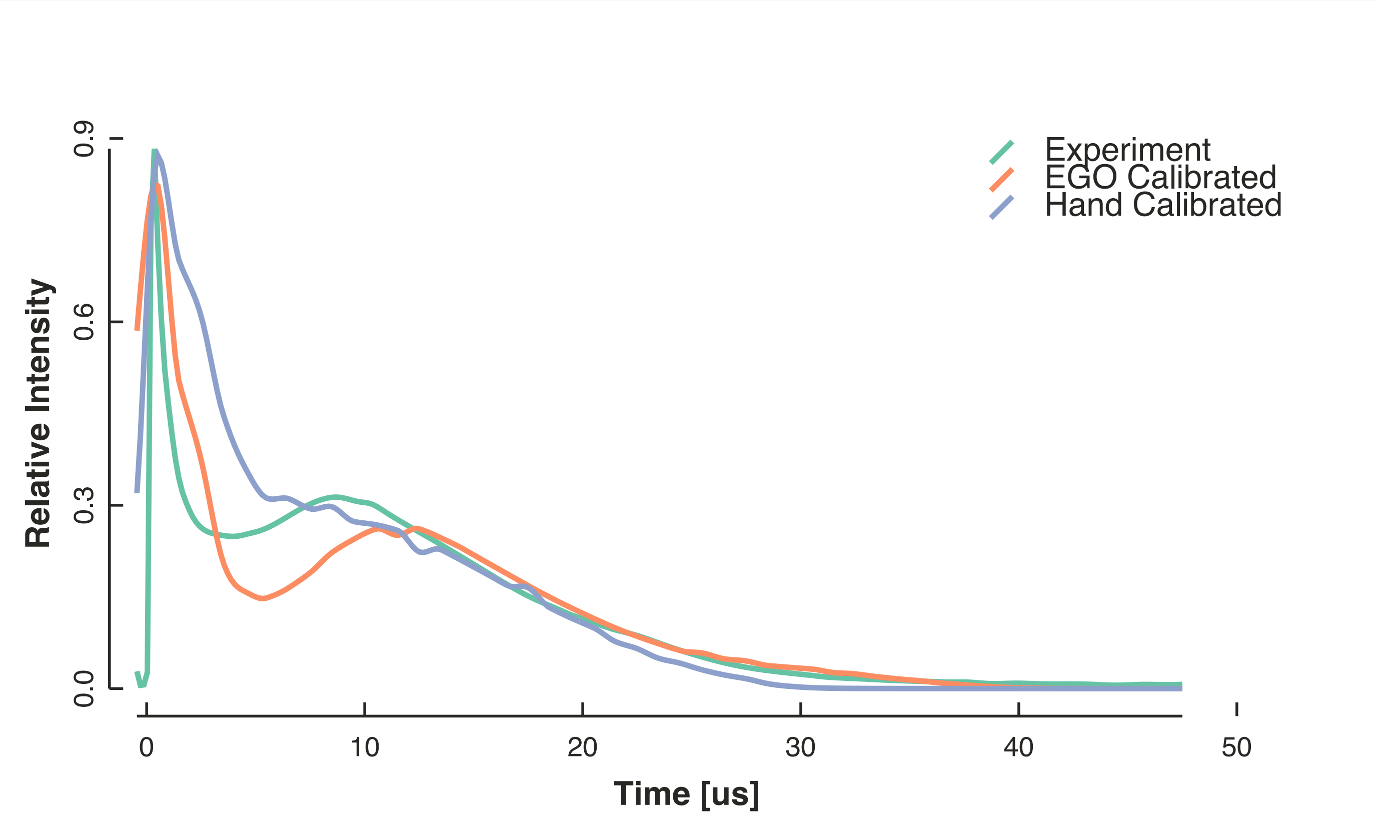
Calibrate a conventional explosion detonator to a computational hydro code developed at SNL

Calibration parameters relate to temperature floor of explosion



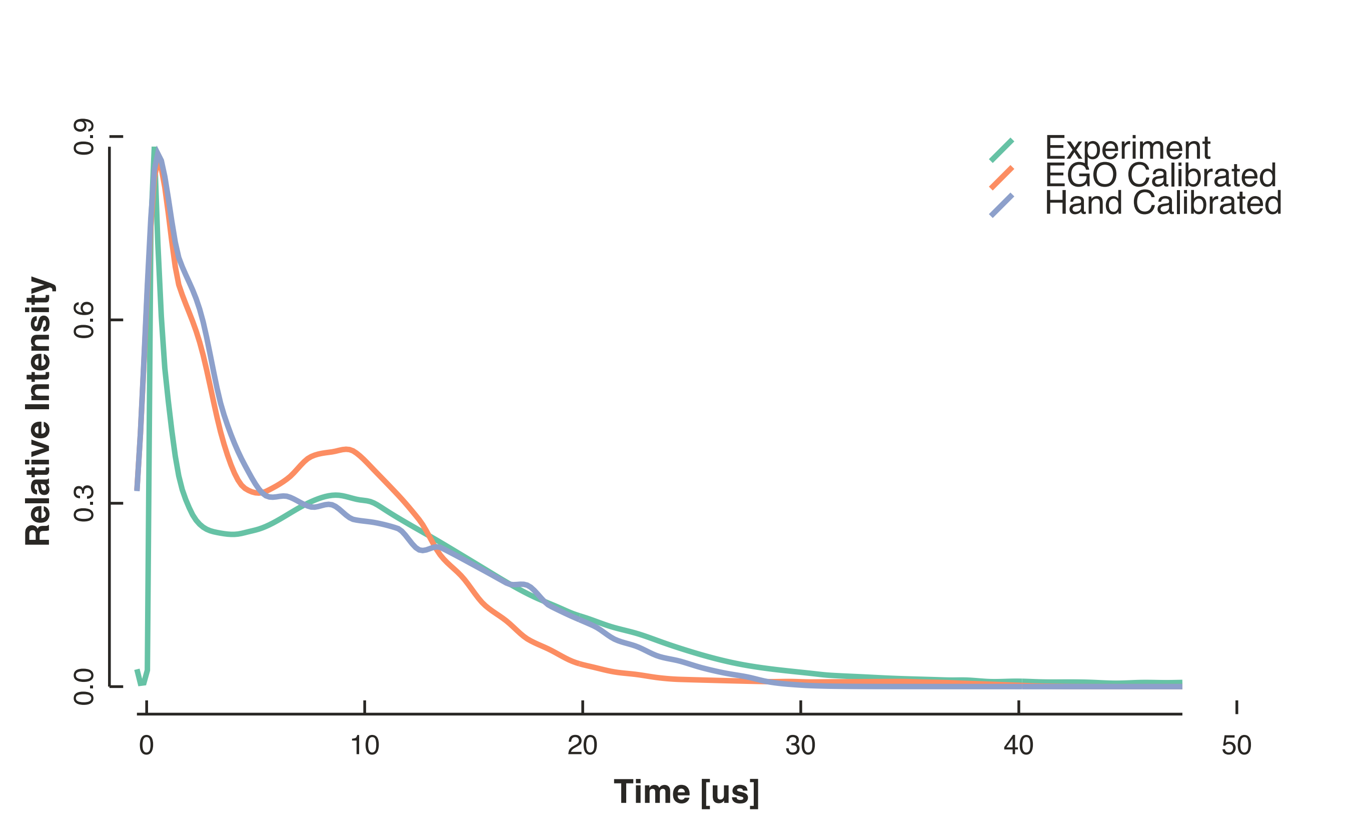
Global Optimization

- Executed a global optimization using Dakota on phase distance
- Due to relative intensities (non calibrated measurements) have a tough time capturing both peaks
  - Multiple local minimum



Local Optimization

- Excited a local optimization using Dakota
  - N2SOL
  - Quasi-Newton Update
- Started from hand calibrated, start to capture shape
  - Still finding local minimum



Conclusions

- Functional metrics provide a global measure of the difference of a function in terms of amplitude and phase
- Integrated elastic functional metrics into Dakota for calibration using global and local optimization
- Demonstrated ability on a conventional explosive calibration problem
- Future Work
  - Move to calibrated data to avoid issues
  - Bayesian model calibration extension (on going work)


Questions?
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