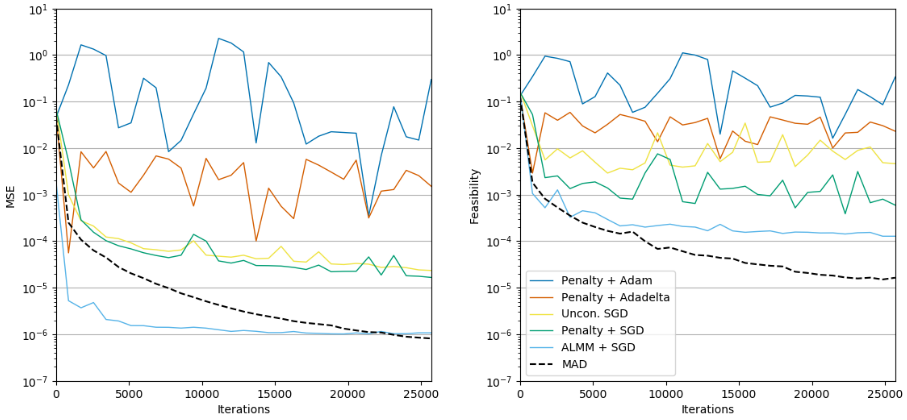
TOWARD CONSTRAINED OPTIMIZATION IN MACHINE LEARNING:

An Error-Tolerant Multisecant Method for Training PINNs



Alp Dener (Presenter)
Argonne National Laboratory

Todd Munson
Argonne National Laboratory

Data and DNN:
M. Andres Miller
R. Michael Churchill
Choong-Seock Chang

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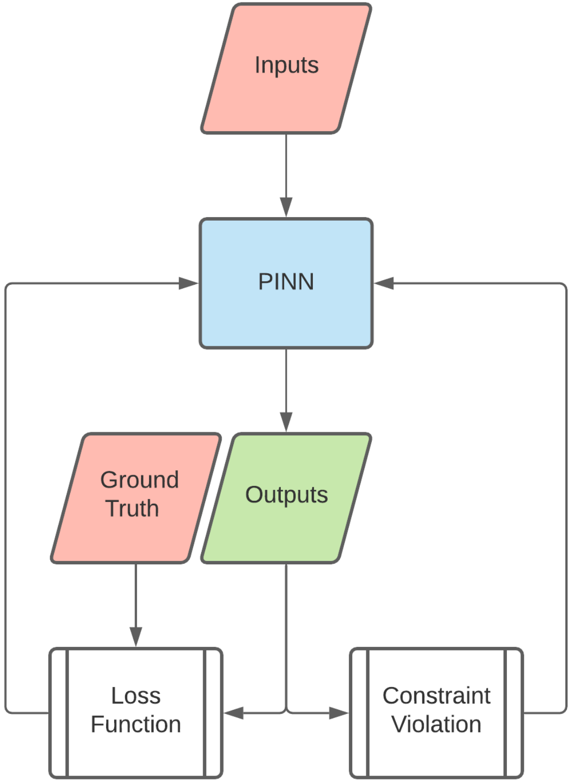
WHAT ARE PINNs?

- "Neural networks trained to solve supervised learning tasks while respecting any given laws of physics…" (Raissi et. al., 2019)

- NNs for approximating physical processes are not new, but most efforts treat NNs as "black box" function estimators

- PINNs seek to incorporate information about the underlying physics into the NN architecture or the training problem



TWO CLASSES OF PINNs…

”Hard” Constrained

NN architecture encodes constraints information

- Untrainable projection layer(s)
  (Mohan et. al., 2020)
- Embedded governing eqns.
  (Raissi et. al., 2019)

Requires knowledge of underlying physics

”Soft” Constrained

Training problem reformulated as constrained optimization

- Penalized loss functions
  (Erichson et. al., 2019)
  (Wu et. al., 2019)
  (Raissi et. al., 2019)

Difficulty tuning penalty term
Feasibility is not guaranteed

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WHY "SOFT" CONSTRAINTS?

Advantages:

- No assumptions about governing equations, quantities of interest, or constraint properties

- Easy to plug-and-play into different applications

- Domain experts do not need to understand ML and vice versa

Challenges:

- State-of-the-art is penalty methods sometimes fail to train! (Wang et. al. 2020)
  - Tuning penalty factors
  - Scaling discrepancies between loss and constraints

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We need better training methods!

OUTLINE

Review

- Training with Constraints
- Dealing with Large Data Sets
- Penalty Methods

Constrained Training

- Sequential Quadratic Programming
- Quasi-Newton Approximations
- Multisecant Method

Test Cases

- MNIST Image Classification Problem (Unconstrained)
- Approximating the Fokker-Planck-Landau Collision Operator

TRAINING WITH CONSTRAINTS

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & \mathcal{J}(x;y) = \|\mathcal{M}(p;y) - \mathcal{R}(y)\|_2^2 \\ \text{subject to} \quad & \mathcal{C}(\mathcal{M}(x;y)) = 0 \end{aligned}$$

- $\mathcal{J}(x; y)$ – mean squared error (MSE) loss function
- $\mathcal{M}(x; y)$ – neural network model
- $\mathcal{C}(\mathcal{M}(x; y))$ – constraints on model output
- x – network weights/parameters
- $\mathcal{R}(y)$ – "ground truth" function/process to be approximated by the network

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`scipy.optimize` can solve a full-batch problem

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DEALING WITH LARGE DATA SETS

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Split the data into randomized batches of size N_b

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & \hat{\mathcal{J}}(x;y) = \frac{1}{N_b} \sum_{i}^{N_b} \|\mathcal{M}(x;y_i) - \mathcal{R}(y_i)\|_2^2 \\ \text{subject to} \quad & \hat{\mathcal{C}}(\mathcal{M}(x;y)) = \frac{1}{N_b} \sum_{i}^{N_b} \mathcal{C}(\mathcal{M}(x;y_i)) = 0 \end{aligned}$$

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Conventional constrained optimization methods cannot solve this!

PENALTY METHODS

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & \hat{\mathcal{J}}(x;y) \\ \text{subject to} \quad & \hat{\mathcal{C}}(\mathcal{M}(x;y)) = 0 \end{aligned}$$

$$\Downarrow$$

$$\underset{x}{\text{minimize}} \quad \hat{\mathcal{J}}(x;y) + \frac{\mu}{2}\|\hat{\mathcal{C}}(\mathcal{M}(x;y))\|_2^2$$

- Add a scalar measure of constraint violation into the loss function
- Converts into unconstrained problem
- ℓ_2-penalty example shown
- Parameter μ determines emphasis on constraint

SEQUENTIAL QUADRATIC PROGRAMMING

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & \hat{\mathcal{J}}(x;y) \\ \text{subject to} \quad & \hat{\mathcal{C}}(\mathcal{M}(x;y)) = 0 \end{aligned}$$

Formulate the Lagrangian: $\mathcal{L} = \hat{\mathcal{J}} + \lambda^T \hat{\mathcal{C}}$

Differentiate for first-order optimality conditions:

$$\begin{aligned} \nabla_x \mathcal{L} = \nabla_x \hat{\mathcal{J}} + \lambda^T \nabla_x \hat{\mathcal{C}} &= 0 \\ \nabla_\lambda \mathcal{L} = \hat{\mathcal{C}} &= 0 \end{aligned}$$

Apply Newton's method:

$$\begin{bmatrix} H & A \\ A^T & 0 \end{bmatrix} \begin{pmatrix} \Delta p \\ \Delta \lambda \end{pmatrix} = \begin{pmatrix} -\nabla_x \mathcal{L} \\ -\hat{\mathcal{C}} \end{pmatrix} \qquad \begin{aligned} H &= \nabla^2_{xx} \mathcal{L} \\ A &= \nabla_x \hat{\mathcal{C}} \end{aligned}$$

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QUASI-NEWTON APPROXIMATIONS

$$W_{k+1} = \begin{cases} \underset{W}{\text{minimize}} & \|W - W_k\| \\ \text{subject to} & W(g_k - g_{k-1}) = x_k - x_{k-1} \end{cases}$$

$$W = \left(\nabla^2_{xx} f(x)\right)^{-1}$$
$$g = \nabla_x f(x)$$

- Quasi-Newton methods iteratively approximate the inverse-Hessian but they do not address constraints
- Cannot compute full-batch constraint Jacobians for large data sets so we need to approximate

Can we approximate the entire matrix (Hessian + constraint Jacobians) using inaccurate first-order information?

MULTISECANT METHOD

- Quasi-Newton methods are based on enforcing the Secant condition on every new iterate/gradient update

$$W_{k+1} = \begin{cases} \underset{W}{\text{minimize}} & \|W - W_k\| \\ \text{subject to} & \boxed{W\Delta g_k = \Delta x_k} \end{cases} \qquad \begin{aligned} W &= \left(\nabla^2_{xx} f(x)\right)^{-1} \\ g &= \nabla_x f(x) \end{aligned}$$

- Multisecant methods construct an approximation by simultaneously enforcing the Secant condition on "q" stored iterates where $\widetilde{W}$ is a "preconditioner"

$$W_k = \begin{cases} \underset{H}{\text{minimize}} & \|W - \tilde{W}\| \\ \text{subject to} & \boxed{WG_k = X_k} \end{cases} \qquad \begin{aligned} X_k &= \begin{bmatrix} \Delta x_{k-q} & \Delta x_{k-q+1} & \dots & \Delta x_{k-1} & \Delta x_k \end{bmatrix} \\ G_k &= \begin{bmatrix} \Delta g_{k-q} & \Delta g_{k-q+1} & \dots & \Delta g_{k-1} & \Delta g_k \end{bmatrix} \end{aligned}$$

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$$G_k = \begin{bmatrix} \Delta g_{k-q} & \Delta g_{k-q+1} & \dots & \Delta g_{k-1} & \Delta g_k \end{bmatrix}$$

- First appearance in material sciences (Vanderbilt and Louie, 1984)
- Formally defined as a “generalized Broyden’s method” equivalent to Anderson mixing with $\widetilde{W} = \alpha I$ (Eyert, 2006)
- Shown to be effective for solving **noisy** nonlinear systems of equations (Bierlaire and Crittin, 2006)
- Adapted to PDE-constrained optimization with inaccurate forward and adjoint solves (Hicken et. al., 2017)

MULTISECANT FOR MACHINE LEARNING?

$$\underset{x}{\text{minimize}} \quad \hat{\mathcal{J}}(x;y) = \frac{1}{N_b}\sum_{i}^{N_b} \|\mathcal{M}(x;y_i) - \mathcal{R}(y_i)\|_2^2$$

$$\text{subject to} \quad \hat{\mathcal{C}}(\mathcal{M}(x;y)) = \frac{1}{N_b}\sum_{i}^{N_b} \mathcal{C}(\mathcal{M}(x;y_i)) = 0$$

Formulate the Lagrangian: $\mathcal{L} = \hat{\mathcal{J}} + \lambda^T \hat{\mathcal{C}}$

Differentiate for first-order optimality conditions:

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This is a "noisy" system of nonlinear equations!

MAD: MULTISECANT ACCELERATED DESCENT

Find (x^*, λ^*) such that: $\begin{bmatrix} \nabla_x \mathcal{L} \\ \nabla_\lambda \mathcal{L} \end{bmatrix} = \begin{bmatrix} \nabla_x \hat{\mathcal{J}}(x^*) + {\lambda^*}^T \nabla_x \hat{\mathcal{C}}(x^*) \\ \hat{\mathcal{C}}(x^*) \end{bmatrix} = \mathbf{0}$

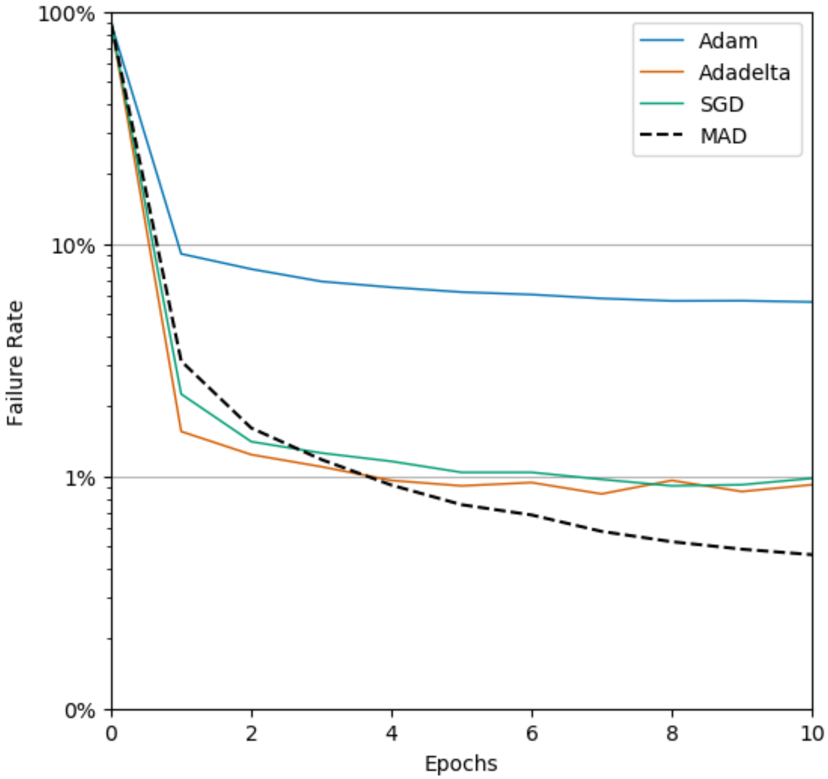
Set $\hat{x}_0 = [x_0, \lambda_0]$ and $g_0 = [\nabla_x \mathcal{L}_0, \nabla_\lambda \mathcal{L}_0]$
Take a gradient descent step $p_1 = p_0 - \eta g_0$
for $k = 1, 2, \ldots$ **do**
  Update X_k and G_k with $(\hat{x}_k - \hat{x}_{k-1})$ and $(g_k - g_{k-1})$
  Solve least squares problem $\gamma = \arg\min_\gamma \|g_k - G_k \gamma\|$
  Compute step direction $\Delta \hat{x}_k = -\tilde{W} g_k - (X_k - \tilde{W} G_k)\gamma$
  Update $\hat{x}_{k+1} = \hat{x}_k + \eta \Delta \hat{x}_k$
end for

TEST CASE: IMAGE CLASSIFICATION

Image source: Josef Steppan (wikimedia.org)

- Handwritten digit classification problem
- 60,000 images for training and 10,000 for testing
- Cloned from pyTorch MNIST example
    - Two Conv2D layers
    - Two fully-connected linear layers
    - Softmax output layer
    - 1,199,882 parameters

TEST CASE: MNIST CLASSIFICATION



	Adam	Adadelta	SGD
Init. LR	1.0	N/A	0.001

- “Reduce LR on plateau” scheduler
- MAD Parameters:

$$q = 10 \qquad \eta_0 = 0.01$$

- pyTorch defaults for others

TEST CASE: XGC FPL COLLISION OPERATOR

- **XGC** is a hybrid Lagrangian-Eulerian particle-in-cell based gyrokinetic code used for simulating the edge region of fusion devices

- Fokker-Planck-Landau (FPL) collision operator in XGC scales quadratically with number of species

Can we accelerate XGC by replacing collision operator with a DNN?

DNN must conserve mass, momentum and energy!

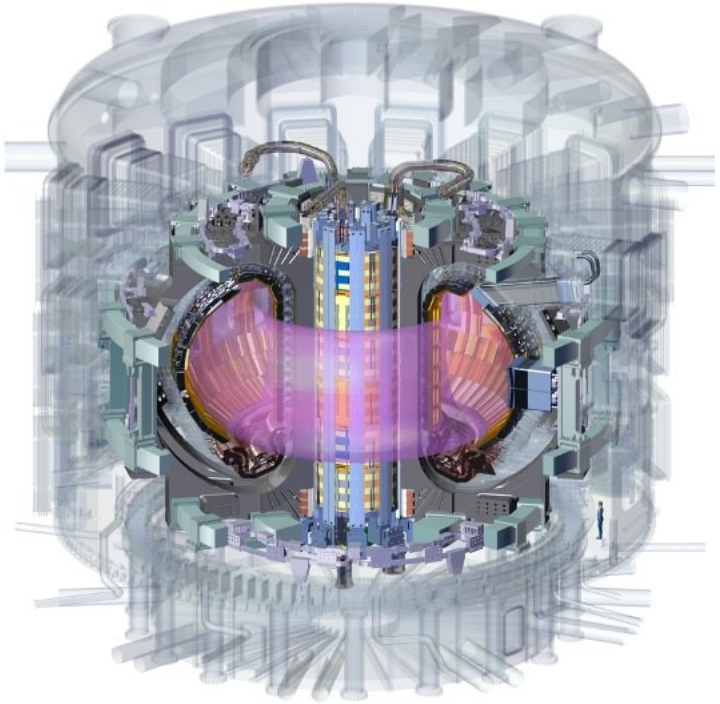
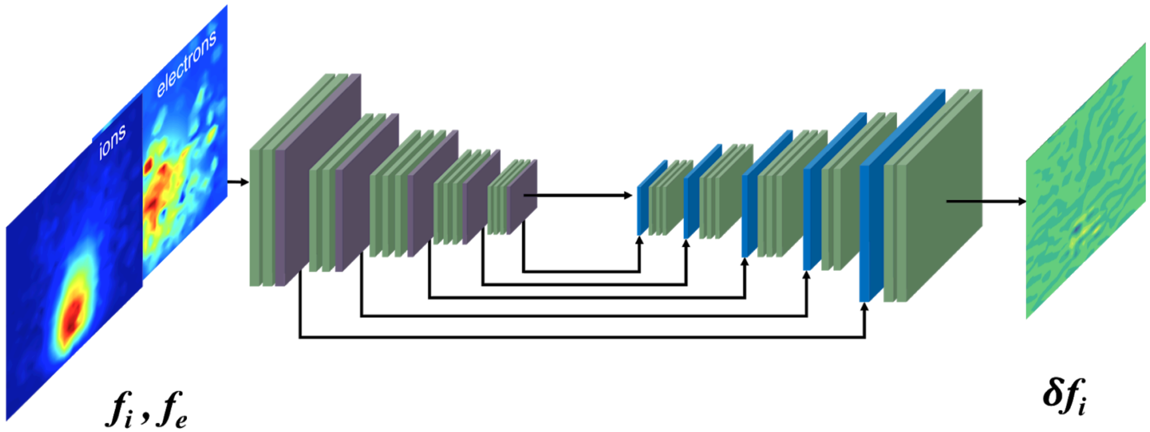


Image Source: iter.org

TEST CASE: XGC FPL COLLISION OPERATOR

- Collision operator computes the change in velocity distribution field of one species (Δf_i) based on the current velocity distributions of all species $(f_i; f_e)$
- Replace FPL collision operator with a ReSeg network (Visin et. al. 2016)

$$\Delta f_i^{ML} = \mathcal{M}(p; f_i^{XGC}; f_e^{XGC})$$



- 2,664,877 parameters
- 96,000 data points for training
- 12,000 data points for validation
- 12,000 data points for out-of-sample testing

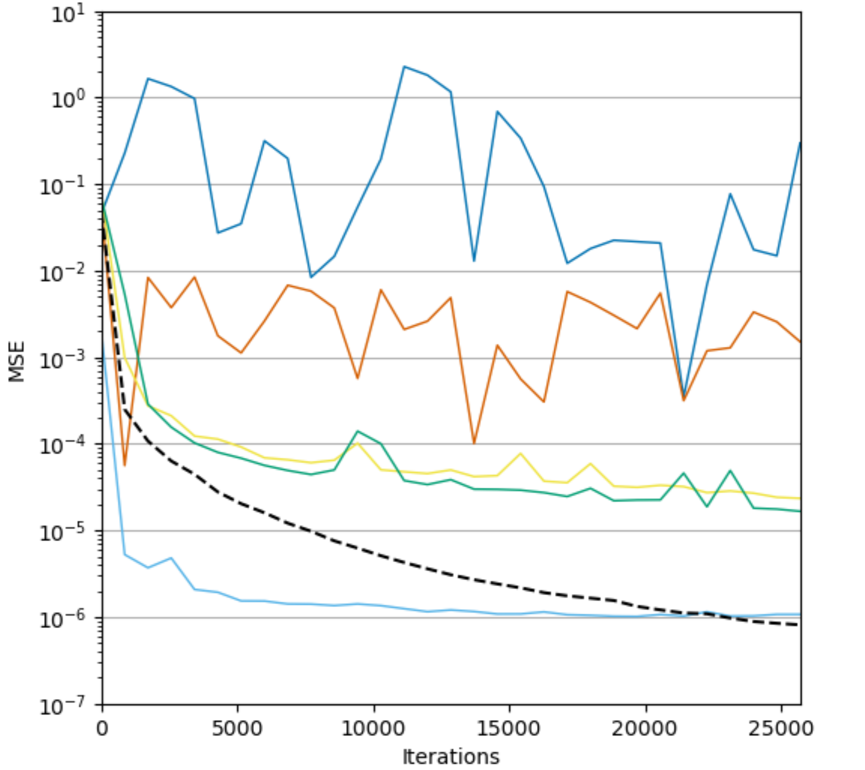
TEST CASE: XGC FPL COLLISION OPERATOR

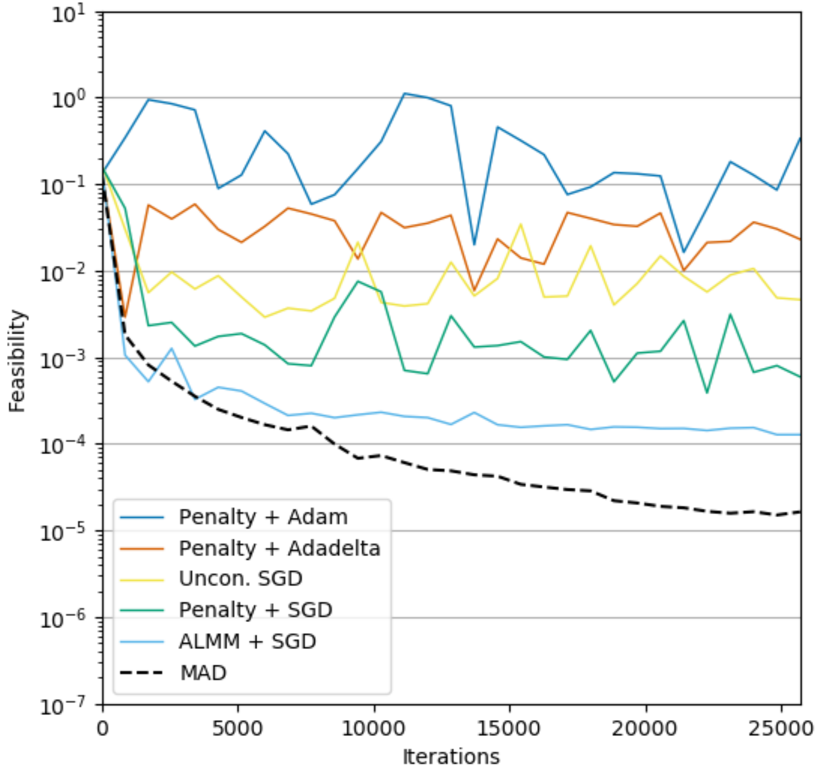
$$\underset{p}{\text{minimize}} \quad \hat{\mathcal{J}}(p) = \frac{1}{2N}\sum_{j}^{N} \|\mathcal{M}(p; f_{i,j}^{XGC}; f_{e,j}^{XGC}) - \Delta f_{i,j}^{XGC}\|_2^2$$

$$\text{subject to} \quad \hat{\mathcal{C}}(p) = \frac{1}{N}\sum_{j}^{N} \begin{pmatrix} \Delta m(\mathcal{M}(p; f_{i,j}^{XGC}; f_{e,j}^{XGC})) \\ \Delta P(\mathcal{M}(p; f_{i,j}^{XGC}; f_{e,j}^{XGC})) \\ \Delta E(\mathcal{M}(p; f_{i,j}^{XGC}; f_{e,j}^{XGC})) \end{pmatrix} = \mathbf{0}$$

- Batch-averaged conservation constraints on mass (m), momentum (P) and energy (E)
- In previous work, we solved this with a stochastic augmented-Lagrangian method of multipliers (Dener et. al., 2020) – see Todd’s talk in MS80
- In current work, we try a different approach with MAD and compare to SALMM as well as a penalty method

TEST CASE: XGC FPL COLLISION OPERATOR





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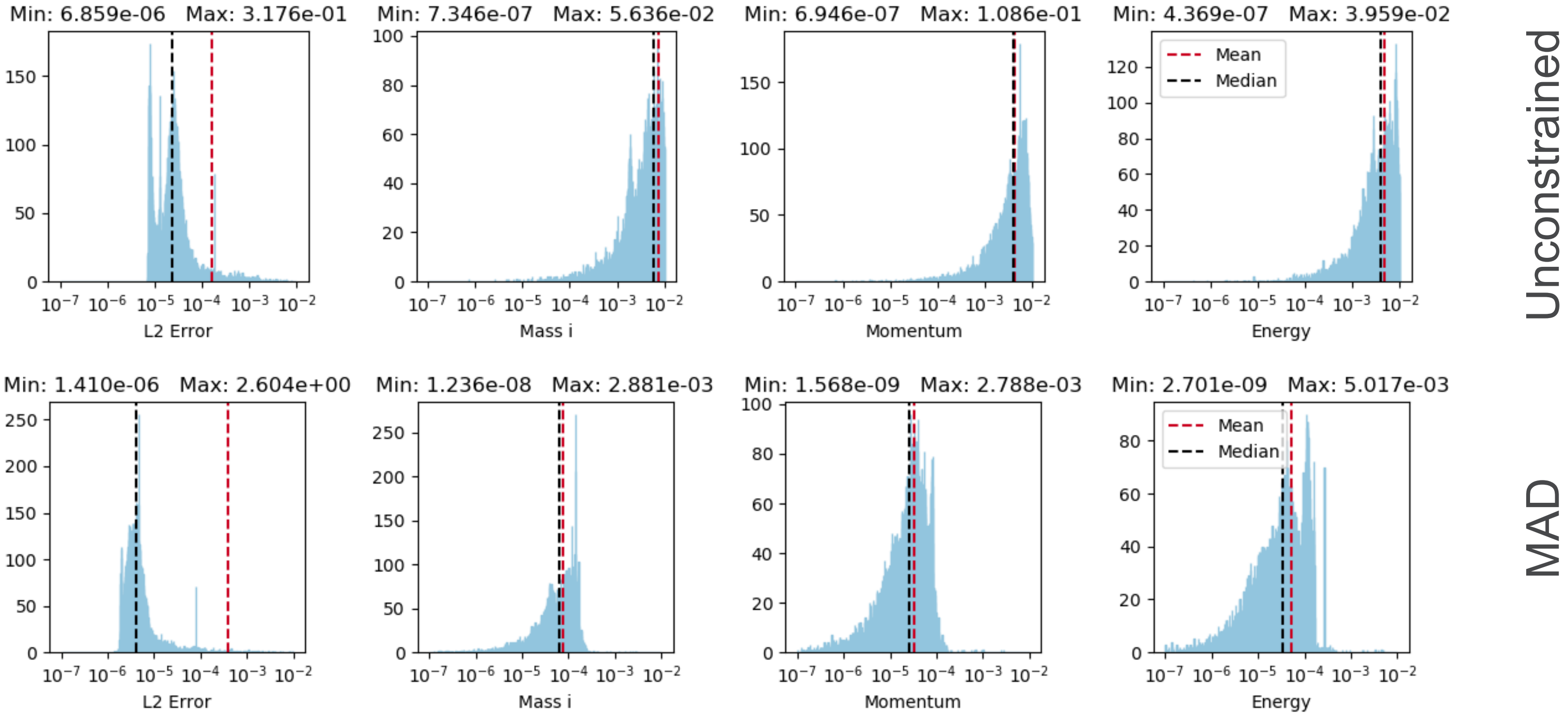

WRAPPING UP…

What did we learn?

- We can and should do better than just penalizing the loss function!
- PINN training methods need to be guided by first-order optimality conditions
- No such thing as parameter-free training, but maybe we can trade hard-to-tune parameters (i.e. the penalty factor) for more benign ones
- Most of this is “old ideas made new again”

Where do we go from here?

- Quasi-Newton Hessian initialization techniques for ”preconditioner” $\widetilde{W}$
- Efficient ways to adapt non-monotone line searches to ML training
- More to learn from literature on solving noisy nonlinear systems of equations
- Visualizing the *constrained* loss landscape (Li et. al., 2018)

RELATED WORKS

Miller, M. A., Churchill, R. M., Dener, A., Chang, C. S., Munson, T., & Hager, R "*Encoder-decoder neural network for solving the nonlinear Fokker-Planck-Landau collision operator in XGC*" arXiv preprint arXiv:2009.06534 (2020)

Dener, A., Miller, M. A., Churchill, R. M., Munson, T., & Chang, C. S. "*Training neural networks under physical constraints using a stochastic augmented Lagrangian approach*" arXiv preprint arXiv:2009.07330 (2020)

Hicken, J. E., Meng, P., & Dener, A. "*Error-tolerant multisecant method for nonlinearly constrained optimization*" arXiv preprint arXiv:1709.06985 (2017)

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The XGC simulations used computational resources at the Argonne (Theta) and Oak Ridge (Summit) Leadership Computing Facilities, DOE Office of Science User Facilities supported under Contracts DE-AC02-06CH11357 and DE-AC05-00OR22725, respectively.