Physics Based Machine Learning for Inverse Problems

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https://github.com/kailaix/ADCME.jl

★ The Pathway to Physics Based Machine Learning ★
Outline

1. Inverse Modeling
2. Automatic Differentiation
3. Physics Constrained Learning
4. Applications
5. Some Perspectives
**Inverse Modeling**

- **Inverse modeling** identifies a certain set of parameters or functions with which the outputs of the forward analysis matches the desired result or measurement.

- Many real life engineering problems can be formulated as inverse modeling problems: shape optimization for improving the performance of structures, optimal control of fluid dynamic systems, etc.
Inverse Modeling

**Forward Problem**
- Model Parameters
- Physical Laws
- Prediction of Observations

**Inverse Problem**
- Observations
- Physical Laws
- Estimation of Parameters
Inverse Modeling

We can formulate inverse modeling as a PDE-constrained optimization problem

$$\min_{\theta} L_h(u_h) \quad \text{s.t.} \quad F_h(\theta, u_h) = 0$$

- The loss function $L_h$ measures the discrepancy between the prediction $u_h$ and the observation $u_{\text{obs}}$, e.g., $L_h(u_h) = \|u_h - u_{\text{obs}}\|_2^2$.
- $\theta$ is the model parameter to be calibrated.
- The physics constraints $F_h(\theta, u_h) = 0$ are described by a system of partial differential equations. Solving for $u_h$ may require solving linear systems or applying an iterative algorithm such as the Newton-Raphson method.
Function Inverse Problem

\[ \min_f L_h(u_h) \quad \text{s.t.} \quad F_h(f, u_h) = 0 \]

What if the unknown is a function instead of a set of parameters?

- Koopman operator in dynamical systems.
- Constitutive relations in solid mechanics.
- Turbulent closure relations in fluid mechanics.
- ...

The candidate solution space is infinite dimensional.
Physics Based Machine Learning

\[
\min_{\theta} L_h(u_h) \quad \text{s.t.} \quad F_h(\text{NN}_\theta, u_h) = 0
\]

- Deep neural networks exhibit capability of approximating high dimensional and complicated functions.

- **Physics based machine learning**: the unknown function is approximated by a deep neural network, and the physical constraints are enforced by numerical schemes.

- Satisfy the physics to the largest extent.

![Diagram showing data, first principles, numerical schemes, and neural networks connected with arrows to illustrate inverse modeling.](image)
Gradient Based Optimization

\[
\min_{\theta} L_h(u_h) \quad \text{s.t.} \quad F_h(\theta, u_h) = 0 \quad (1)
\]

- We can now apply a gradient-based optimization method to (1).
- The key is to calculate the gradient descent direction \( g^k \)

\[
\theta^{k+1} \leftarrow \theta^k - \alpha g^k
\]
Automatic Differentiation

The fact that bridges the technical gap between machine learning and inverse modeling:

- Deep learning (and many other machine learning techniques) and numerical schemes share the same computational model: composition of individual operators.

Mathematical Fact

Back-propagation

Reverse-mode

Automatic Differentiation

Discrete

Adjoint-State Method
A computational graph is a functional description of the required computation. In the computational graph, an edge represents data, such as a scalar, a vector, a matrix or a tensor. A node represents a function (operator) whose input arguments are the incoming edges and output values are the outcoming edges.

How to build a computational graph for $z = \sin(x_1 + x_2) + x_2^2 x_3$?
Reverse Mode AD

\[
\frac{df(g(x))}{dx} = f'(g(x))g'(x)
\]

- Computing in the reverse order of forward computation.
- Each node in the computational graph
  - Aggregates all the gradients from downstreams
  - Back-propagates the gradient to upstream nodes.
Example: Reverse Mode AD

\[ z = \sin(x_1 + x_2) + x_2^2x_3 \]
Example: Reverse Mode AD

\[ z = \sin(x_1 + x_2) + x_2^2 x_3 \]
Example: Reverse Mode AD

\[ z = \sin(x_1 + x_2) + x_2^2 x_3 \]
Example: Reverse Mode AD

\[ z = \sin(x_1 + x_2) + x_2^2 x_3 \]
The forward-mode automatic differentiation uses the chain rule to propagate the gradients.

\[
\frac{\partial f \circ g(x)}{\partial x} = f'(g(x))g'(x)
\]

- Compute in the same order as function evaluation.
- Each node in the computational graph
  - Aggregate all the gradients from up-streams.
  - Forward the gradient to down-stream nodes.
Example: Forward Mode AD

Let's consider a specific way for computing

\[ f(x) = \begin{bmatrix} x^4 \\ x^2 + \sin(x) \\ -\sin(x) \end{bmatrix} \]

\[
\begin{align*}
y_3 &= y_1^2 \\
y_4 &= y_1 + y_2 \\
y_5 &= -y_2
\end{align*}
\]

\[
\begin{align*}
(y_1, y'_1) &= (x^2, 2x) \\
(y_2, y'_2) &= (\sin x, \cos x)
\end{align*}
\]

\[
\begin{align*}
(y_3, y'_3) &= (y_1^2, 2y_1y'_1) = (x^4, 4x^3) \\
(y_4, y'_4) &= (y_1 + y_1, y'_1 + y'_2) \\
&= (x^2 + \sin x, 2x + \cos x) \\
(y_5, y'_5) &= (-y_2, -y'_2) = (-\sin x, -\cos x)
\end{align*}
\]
In general, for a function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$

<table>
<thead>
<tr>
<th>Mode</th>
<th>Suitable for ...</th>
<th>Complexity$^1$</th>
<th>Application</th>
</tr>
</thead>
<tbody>
<tr>
<td>Forward</td>
<td>$m \gg n$</td>
<td>$\leq 2.5$ OPS($f(x)$)</td>
<td>UQ</td>
</tr>
<tr>
<td>Reverse</td>
<td>$m \ll n$</td>
<td>$\leq 4$ OPS($f(x)$)</td>
<td>Inverse Modeling</td>
</tr>
</tbody>
</table>

There are also many other interesting topics
- Mixed mode AD: many-to-many mappings.
- Computing sparse Jacobian matrices using AD by exploiting sparse structures.


$^1$OPS is a metric for complexity in terms of fused-multiply adds.
To leverage automatic differentiation for inverse modeling, we need to express the numerical schemes in the “AD language”: computational graph.

No matter how complicated a numerical scheme is, it can be decomposed into a collection of operators that are interlinked via state variable dependencies.
Consider a concrete PDE-constrained optimization problem:

\[
\begin{align*}
\min_{u_1, \theta} & \quad J = f_4(u_1, u_2, u_3, u_4), \\
\text{s.t.} & \quad u_2 = f_1(u_1, \theta), \\
& \quad u_3 = f_2(u_2, \theta), \\
& \quad u_4 = f_3(u_3, \theta).
\end{align*}
\]

- \(f_1, f_2, f_3\) are PDE constraints
- \(f_4\) is the loss function
- \(u_1\) is the initial condition
- \(\theta\) is the model parameter
The Relationship between reverse-mode Automatic Differentiation and KKT Condition

Solving the constrained optimization method using adjoint-state methods:

- The Lagrange multiplier is

\[ \mathcal{L} = f_4(u_1, u_2, u_3, u_4) + \lambda_2^T (f_1(u_1, \theta) - u_2) + \lambda_3^T (f_2(u_2, \theta) - u_3) + \lambda_4^T (f_3(u_3, \theta) - u_4) \]

- Therefore, the first order KKT condition of the constrained PDE system is

\[
\begin{align*}
\lambda_4^T &= \frac{\partial f_4}{\partial u_4} \\
\lambda_3^T &= \frac{\partial f_4}{\partial u_3} + \lambda_4^T \frac{\partial f_3}{\partial u_3} \\
\lambda_2^T &= \frac{\partial f_4}{\partial u_2} + \lambda_3^T \frac{\partial f_2}{\partial u_2} \\
\frac{\partial \mathcal{L}}{\partial \theta} &= \lambda_2^T \frac{\partial f_1}{\partial \theta} + \lambda_3^T \frac{\partial f_2}{\partial \theta} + \lambda_4^T \frac{\partial f_3}{\partial \theta} \Rightarrow \text{Sensitivity } \frac{\partial J}{\partial \theta}
\end{align*}
\]
The Relationship between reverse-mode Automatic Differentiation and KKT Condition

How do we implement reverse-mode automatic differentiation for computing the gradients?

- Consider the operator $f_2$, we need to implement two operators

  Forward: $u_3 = f_2(u_2, \theta)$

  Backward: $\frac{\partial J}{\partial u_2}, \frac{\partial J}{\partial \theta} = b_2 \left( \frac{\partial J^{\text{tot}}}{\partial u_3}, u_2, \theta \right)$

  $\frac{\partial J^{\text{tot}}}{\partial u_3}$ is the “total” gradient $u_3$ received from the downstream in the computational graph.

- The backward operator is implemented using the chain rule

  $$\frac{\partial J}{\partial u_2} = \frac{\partial J^{\text{tot}}}{\partial u_3} \frac{\partial f_2}{\partial u_2} \quad \frac{\partial J}{\partial \theta} = \frac{\partial J^{\text{tot}}}{\partial u_3} \frac{\partial f_2}{\partial \theta}$$

What are $\frac{\partial J}{\partial u_2}$, $\frac{\partial J}{\partial \theta}$, and $\frac{\partial J^{\text{tot}}}{\partial u_3}$ exactly?
The Relationship between reverse-mode Automatic Differentiation and KKT Condition

The total gradient $u_2$ received is

$$\frac{\partial J^{\text{tot}}}{\partial u_2} = \frac{\partial f_4}{\partial u_2} + \frac{\partial J}{\partial u_2} = \frac{\partial f_4}{\partial u_2} + \frac{\partial J^{\text{tot}}}{\partial u_3} \frac{\partial f_2}{\partial u_2}$$

The dual constraint in the KKT condition

$$\lambda_2^T = \frac{\partial f_4}{\partial u_2} + \lambda_3^T \frac{\partial f_2}{\partial u_2}$$

The following equality can be verified

$$\lambda_i^T = \frac{\partial J^{\text{tot}}}{\partial u_i}$$

In general, the reverse-mode AD is back-propagating the Lagrange multiplier (adjoint variables).
The Relationship between reverse-mode Automatic Differentiation and KKT Condition

- The well-established adjoint-state method is equivalent to solving the KKT system.
- The adjoint-state methods are challenging to implement, mainly due to the time-consuming and difficult process of deriving the gradients of a complex system.
- Using reverse-mode automatic differentiation is equivalent to solving the inverse modeling problem using discrete adjoint-state methods, but in a more manageable way.
- Computational graph based implementation also allows for automatic compilation time optimization and parallelization.
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2. Automatic Differentiation
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5. Some Perspectives
Challenges in AD

- Most AD frameworks only deal with explicit operators, i.e., the functions that have analytical derivatives, or composition of these functions.
- Many scientific computing algorithms are iterative or implicit in nature.

<table>
<thead>
<tr>
<th>Linear/Nonlinear</th>
<th>Explicit/Implicit</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear</td>
<td>Explicit</td>
<td>$y = Ax$</td>
</tr>
<tr>
<td>Nonlinear</td>
<td>Explicit</td>
<td>$y = F(x)$</td>
</tr>
<tr>
<td><strong>Linear</strong></td>
<td><strong>Implicit</strong></td>
<td>$Ay = x$</td>
</tr>
<tr>
<td>Nonlinear</td>
<td>Implicit</td>
<td>$F(x, y) = 0$</td>
</tr>
</tbody>
</table>
An efficient way to do automatic differentiation is to apply the implicit function theorem. For our example, \( F(x, y) = x^3 - (y^3 + y) = 0 \); treat \( y \) as a function of \( x \) and take the derivative on both sides

\[
3x^2 - 3y(x)^2 y'(x) - y'(x) = 0 \Rightarrow y'(x) = \frac{3x^2}{3y^2 + 1}
\]

The above gradient is exact.

Can we apply the same idea to inverse modeling?
An efficient way is to apply the implicit function theorem. For our example, \( F(x, y) = x^3 - (y^3 + y) = 0 \), treat \( y \) as a function of \( x \) and take the derivative on both sides

\[
3x^2 - 3y(x)^2 y'(x) - 1 = 0 \implies y'(x) = \frac{3x^2 - 1}{3y(x)^2}
\]

The above gradient is exact.

**Can we apply the same idea to inverse modeling?**
Physics Constrained Learning

$$\min_{\theta} L_h(u_h) \quad \text{s.t.} \quad F_h(\theta, u_h) = 0$$

- Assume that we solve for $u_h = G_h(\theta)$ with $F_h(\theta, u_h) = 0$, and then
  $$\tilde{L}_h(\theta) = L_h(G_h(\theta))$$

- Applying the implicit function theorem
  $$\frac{\partial F_h(\theta, u_h)}{\partial \theta} + \frac{\partial F_h(\theta, u_h)}{\partial u_h} \frac{\partial G_h(\theta)}{\partial \theta} = 0 \Rightarrow \frac{\partial G_h(\theta)}{\partial \theta} = -\left(\frac{\partial F_h(\theta, u_h)}{\partial u_h}\right)^{-1} \frac{\partial F_h(\theta, u_h)}{\partial \theta}$$

- Finally we have
  $$\frac{\partial \tilde{L}_h(\theta)}{\partial \theta} = \frac{\partial L_h(u_h)}{\partial u_h} \frac{\partial G_h(\theta)}{\partial \theta} = -\frac{\partial L_h(u_h)}{\partial u_h} \left(\frac{\partial F_h(\theta, u_h)}{\partial u_h}\right)_{u_h=G_h(\theta)}^{-1} \frac{\partial F_h(\theta, u_h)}{\partial \theta} \bigg|_{u_h=G_h(\theta)}$$
Physics Constrained Learning

\[
\frac{\partial \tilde{L}_h(\theta)}{\partial \theta} = -\frac{\partial L_h(u_h)}{\partial u_h} \left( \frac{\partial F_h(\theta, u_h)}{\partial u_h} \bigg|_{u_h=G_h(\theta)} \right)^{-1} \frac{\partial F_h(\theta, u_h)}{\partial \theta} \bigg|_{u_h=G_h(\theta)}
\]

Step 1: Calculate \( w \) by solving a linear system (never invert the matrix!)

\[
w^T = \frac{\partial L_h(u_h)}{\partial u_h} \left( \frac{\partial F_h}{\partial u_h} \bigg|_{u_h=G_h(\theta)} \right)^{-1}
\]

\[
\begin{array}{c}
1 \times N \\
N \times N
\end{array}
\]

Step 2: Calculate the gradient by automatic differentiation

\[
w^T \frac{\partial F_h}{\partial \theta} \bigg|_{u_h=G_h(\theta)} = \frac{\partial (w^T F_h(\theta, u_h))}{\partial \theta} \bigg|_{u_h=G_h(\theta)}
\]

ADCME

Physics Based Machine Learning

31 / 60
Physics Constrained Learning

Let us consider an example:

\[
\min_{\theta} L(\theta) = \| u_\theta - u_0 \|^2 \\
\text{s.t. } B(\theta)u = y
\]  

(2)

Let \( u_\theta \) denotes the solution to the PDE constraint (assume boundary conditions have been considered in the linear system, e.g., via static condensation).

\[ \tilde{L}(\theta) = \| u_\theta - u_0 \|^2 \]
Physics Constrained Learning

1. \[
\frac{\partial \tilde{L}_h(\theta)}{\partial \theta} = 2(u_\theta - u_0)^T \frac{\partial u_\theta}{\partial \theta}
\]

2. To compute \(\frac{\partial u_\theta}{\partial \theta}\), consider the PDE constraint (\(\theta\) is a scalar)

\[
B(\theta)u_\theta = y
\]

Take the derivative with respect to \(\theta\) on both sides

\[
\frac{\partial B(\theta)}{\partial \theta} u_\theta + B(\theta) \frac{\partial u_\theta}{\partial \theta} = 0 \Rightarrow \frac{\partial u_\theta}{\partial \theta} = -B(\theta)^{-1} \frac{\partial B(\theta)}{\partial \theta} u_\theta
\]

3. Finally,

\[
\frac{\partial \tilde{L}_h(\theta)}{\partial \theta} = -2(u_\theta - u_0)^T B(\theta)^{-1} \frac{\partial B(\theta)}{\partial \theta} u_\theta
\]
Physics Constrained Learning

1. Remember: in reverse-mode AD, gradients are always back-propagated from downstream (objective function) to upstream (unknowns).

2. The following quantity is computed first:

\[ g^T = 2(u_\theta - u_0)^T B(\theta)^{-1} \]

which is equivalent to solve a linear system

\[ B(\theta)^T g = 2(u_\theta - u_0) \]

3. In the gradient back-propagation step, a linear system with an adjoint matrix (compared to the forward computation) is solved.

4. Finally,

\[ \frac{\partial \tilde{L}_h(\theta)}{\partial \theta} = -2(u_\theta - u_0)^T B(\theta)^{-1} \frac{\partial B(\theta)}{\partial \theta} u_\theta = -g^T \frac{\partial B(\theta)}{\partial \theta} u_\theta \]
A trick for evaluating $g^T Bu_\theta$: consider $g$ and $u_\theta$ as independent of $\theta$ in the computational graph, then

$$g^T \frac{\partial B(\theta)}{\partial \theta} u_\theta = \frac{\partial (g^T B(\theta) u_\theta)}{\partial \theta}$$

$g^T B(\theta) u_\theta$ is a scalar, thus we can apply reverse-mode AD to compute $\frac{\partial (g^T B(\theta) u_\theta)}{\partial \theta}$.

Declaring independence of variables can be done with `tf.stop_gradient` in TensorFlow or `independent` in ADCME.
Methodology Summary

Predicted Data
Observed Data
Loss Function
Calculate Gradients
Update Model Parameters

PDE
Initial and Boundary Conditions

Optimizer
Automatic Differentiation
Physics Constrained Learning

Neural Network
Kernel Functions
Physical Parameters
Random Variables
…….
Physics Constrained Learning: Linear System

- Many physical simulations require solving a linear system
  \[ A(\theta_2) u_h = \theta_1 \]

- The corresponding PDE constraint in our formulation is
  \[ F_h(\theta_1, \theta_2, u_h) = \theta_1 - A(\theta_2) u_h = 0 \]

- The backpropagation formula
  \[
  p := \frac{\partial \tilde{L}_h(\theta_1, \theta_2)}{\partial \theta_1} = \frac{\partial L_h(u_h)}{\partial u_h} A(\theta_2)^{-1} \\
  q := \frac{\partial \tilde{L}_h(\theta_1, \theta_2)}{\partial \theta_2} = - \frac{\partial L_h(u_h)}{\partial u_h} A(\theta_2)^{-1} \frac{\partial A(\theta_2)}{\partial \theta_2}
  \]
  which is equivalent to
  \[
  A^T p^T = \left( \frac{\partial L_h(u_h)}{\partial u_h} \right)^T q = -p \frac{\partial A(\theta_2)}{\partial \theta_2}
  \]
Methodology Summary

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Physics Constrained Learning

Physics Based Machine Learning

Neural Network

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Physical Parameters

Random Variables

……

Initial and Boundary Conditions
Outline

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4. Applications
5. Some Perspectives
Many seismic inversion problems can be solved within a unified framework.
The earthquake source function is parameterized by \((g(t) \text{ and } x_0 \text{ are unknowns})\)

\[
f(x, t) = \frac{g(t)}{2\pi\sigma^2} \exp \left( -\frac{||x - x_0||^2}{2\sigma^2} \right)
\]
ADCME makes the heterogeneous computation capability of TensorFlow available for scientific computing.
\[ \sigma_{ij,j} + \rho \ b_i = \rho \ \ddot{u}_i \]

\[ \varepsilon_{ij} = \frac{1}{2}(u_{j,i} + u_{i,j}) \]  

**Observable**: external/body force \( b_i \), displacements \( u_i \) (strains \( \varepsilon_{ij} \) can be computed from \( u_i \)); density \( \rho \) is known.

**Unobservable**: stress \( \sigma_{ij} \).

**Data-driven Constitutive Relations**: modeling the strain-stress relation using a neural network

\[ \text{stress} = M_\theta(\text{strain}, \ldots) \]  

and the neural network is trained by coupling (1) and (2).
Proper form of constitutive relation is crucial for numerical stability

- Elasticity $\Rightarrow \sigma = C_\theta \epsilon$

- Hyperelasticity $\Rightarrow \begin{cases} \sigma = M_\theta(\epsilon) \\ \sigma^{n+1} = L_\theta(\epsilon^{n+1})L_\theta(\epsilon^{n+1})^T(\epsilon^{n+1} - \epsilon^n) + \sigma^n \end{cases}$ (Static)

- Elasto-Plasticity $\Rightarrow \sigma^{n+1} = L_\theta(\epsilon^{n+1}, \epsilon^n, \sigma^n)L_\theta(\epsilon^{n+1}, \epsilon^n, \sigma^n)^T(\epsilon^{n+1} - \epsilon^n) + \sigma^n$

- Weak convexity: $L_\theta L_\theta^T \succ 0$

- Time consistency: $\sigma^{n+1} \rightarrow \sigma^n$ when $\epsilon^{n+1} \rightarrow \epsilon^n$
NNFEM.jl: Robust Constitutive Modeling

- Weak form of balance equations of linear momentum
  \[
  P_i(\theta) = \int_V \rho \ddot{u}_i \delta u_i dVt + \int_V \sigma_{ij}(\theta) \delta \varepsilon_{ij} dV
  \]

  embedded neural network

  \[
  F_i = \int_V \rho b_i \delta u_i dV + \int_{\partial V} t_i \delta u_i dS
  \]

- Train the neural network by
  \[
  L(\theta) = \min_{\theta} \sum_{i=1}^{N} (P_i(\theta) - F_i)^2
  \]

  The gradient \( \nabla L(\theta) \) is computed via automatic differentiation.
NNFEM.jl: Robustic Constitutive Modeling

Piecewise Linear

Neural Network

Radial Basis Functions
vs.
Neural Network

Radial Basis Function Networks
vs.
Neural Network

ADCME
Physics Based Machine Learning
Comparison of different neural network architectures

\[
\sigma^{n+1} = L_\theta(\epsilon^{n+1}, \epsilon^n, \sigma^n) L_\theta(\epsilon^{n+1}, \epsilon^n, \sigma^n)^T (\epsilon^{n+1} - \epsilon^n) + \sigma^n
\]

\[
\sigma^{n+1} = \text{NN}_\theta(\epsilon^{n+1}, \epsilon^n, \sigma^n)
\]

\[
\sigma^{n+1} = \text{NN}_\theta(\epsilon^{n+1}, \epsilon^n, \sigma^n) + \sigma^n
\]
FwiFlow.jl: Elastic Full Waveform Inversion for subsurface flow problems

Observed data
Seismic response
Rocks bulk modulus
CO\textsubscript{2} saturation
Permeability

\[ \frac{dm}{dt} = A(m; K) \]

Forward simulation
Back-Propagation
FwiFlow.jl: Fully Nonlinear Implicit Schemes

- The governing equation is a nonlinear PDE

\[
\frac{\partial}{\partial t} (\phi S_i \rho_i) + \nabla \cdot (\rho_i \nu_i) = \rho_i q_i, \quad i = 1, 2
\]

\[S_1 + S_2 = 1\]

\[\nu_i = -\frac{K k_{ri}}{\tilde{\mu}_i} (\nabla P_i - g \rho_i \nabla Z), \quad i = 1, 2\]

\[k_{r1}(S_1) = \frac{k^o_{r1} S_1^{L1}}{S_1^{L1} + E_1 S_2^{T1}}\]

\[k_{r2}(S_1) = \frac{S_2^{L2}}{S_2^{L2} + E_2 S_1^{T2}}\]

- For stability and efficiency, implicit methods are the industrial standards.

\[
\phi(S_2^{n+1} - S_2^n) - \nabla \cdot (m_2(S_2^{n+1}) K \nabla \psi_2^n) \Delta t = \left( q_2^n + q_1^n \frac{m_2(S_2^{n+1})}{m_1(S_2^{n+1})} \right) \Delta t \quad m_i(s) = \frac{k_{ri}(s)}{\tilde{\mu}_i}
\]

- It is impossible to express the numerical scheme directly in an AD framework. Physics constrained learning is used to enhance the AD framework for computing gradients.
FwiFlow.jl: Showcase

- Task 1: Estimating the permeability from seismic data
  B.C. + Two-Phase Flow Equation + Wave Equation ⇒ Seismic Data

- Task 2: Learning the rock physics model from sparse saturation data.
  The rock physics model is approximated by neural networks
  \[ f_1(S_1; \theta_1) \approx k_{r1}(S_1) \quad f_2(S_1; \theta_2) \approx k_{r2}(S_1) \]
FwiFlow.jl: Showcase

- Task 3: Learning the nonlocal (space or time) hidden dynamics from seismic data. This is very challenging using traditional methods (e.g., the adjoint-state method) because the dynamics is history dependent.

B.C. + Time-/Space-fractional PDE + Wave Equation ⇒ Seismic Data

<table>
<thead>
<tr>
<th>Governing Equation</th>
<th>$\sigma = 0$</th>
<th>$\sigma = 5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_0 D_t^{0.8} m = 10\Delta m$</td>
<td>$a/a^* = 1.0000$</td>
<td>$a/a^* = 0.9109$</td>
</tr>
<tr>
<td></td>
<td>$\alpha = 0.8000$</td>
<td>$\alpha = 0.7993$</td>
</tr>
<tr>
<td>$C_0 D_t^{0.2} m = 10\Delta m$</td>
<td>$a/a^* = 0.9994$</td>
<td>$a/a^* = 0.3474$</td>
</tr>
<tr>
<td></td>
<td>$\alpha = 0.2000$</td>
<td>$\alpha = 0.1826$</td>
</tr>
<tr>
<td>$\frac{\partial m}{\partial t} = -10(-\Delta)^{0.2} m$</td>
<td>$a/a^* = 1.0000$</td>
<td>$a/a^* = 1.0378$</td>
</tr>
<tr>
<td></td>
<td>$s = 0.2000$</td>
<td>$s = 0.2069$</td>
</tr>
<tr>
<td>$\frac{\partial m}{\partial t} = -10(-\Delta)^{0.8} m$</td>
<td>$a/a^* = 1.0000$</td>
<td>$a/a^* = 1.0365$</td>
</tr>
<tr>
<td></td>
<td>$s = 0.8000$</td>
<td>$s = 0.8093$</td>
</tr>
</tbody>
</table>
PoreFlow.jl: Inverse Modeling of Viscoelasticity

- Multi-physics Interaction of Coupled Geomechanics and Multi-Phase Flow Equations

\[
\begin{align*}
\text{div}\sigma(u) - b\nabla p &= 0 \\
\frac{1}{M} \frac{\partial p}{\partial t} + b \frac{\partial \varepsilon_v(u)}{\partial t} - \nabla \cdot \left( \frac{k}{B_f \mu} \nabla p \right) &= f(x, t) \\
\sigma &= \sigma(\varepsilon, \dot{\varepsilon})
\end{align*}
\]

- Approximate the constitutive relation by a neural network

\[
\sigma^{n+1} - \sigma^n = \mathcal{N}\mathcal{N}_\theta(\sigma^n, \varepsilon^n) + H(\varepsilon^{n+1} - \varepsilon^n)
\]
Comparison with space varying linear elasticity approximation

\[ \sigma = H(x, y) \epsilon \] (5)

- Space Varying Linear Elasticity
- NN
- True
PoreFlow.jl: Inverse Modeling of Viscoelasticity

(a) Space Varying Linear Elasticity

(b) NN-based Viscoelasticity
Outline

1. Inverse Modeling
2. Automatic Differentiation
3. Physics Constrained Learning
4. Applications
5. Some Perspectives
Most inverse modeling problems can be classified into 4 categories. To be more concrete, consider the PDE for describing physics

\[ \nabla \cdot (\theta \nabla u(x)) = 0 \quad \mathcal{BC}(u(x)) = 0 \]  

(6)

We observe some quantities depending on the solution \( u \) and want to estimate \( \theta \).

<table>
<thead>
<tr>
<th>Expression</th>
<th>Description</th>
<th>ADCME Solution</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \nabla \cdot (c \nabla u(x)) = 0 )</td>
<td>Parameter Inverse Problem</td>
<td>Discrete Adjoint State Method</td>
<td>( c ) is the minimizer of the error functional</td>
</tr>
<tr>
<td>( \nabla \cdot (f(x) \nabla u(x)) = 0 )</td>
<td>Function Inverse Problem</td>
<td>Neural Network Functional Approximator</td>
<td>( f(x) \approx f_w(x) )</td>
</tr>
<tr>
<td>( \nabla \cdot (f(u) \nabla u(x)) = 0 )</td>
<td>Relation Inverse Problem</td>
<td>Residual Learning Physics Constrained Learning</td>
<td>( f(u) \approx f_w(u) )</td>
</tr>
<tr>
<td>( \nabla \cdot (\omega \nabla u(x)) = 0 )</td>
<td>Stochastic Inverse Problem</td>
<td>Generative Neural Networks</td>
<td>( \omega = f_w(v_{latent}) )</td>
</tr>
</tbody>
</table>

1. Deep neural networks provide a novel function approximator that outperforms traditional basis functions in certain scenarios.

2. Numerical PDEs are not on the opposite side of machine learning. By expressing the known physical constraints using numerical schemes and approximating the unknown with machine learning models, we combine the best of the two worlds, leading to efficient and accurate inverse modeling tools.

Automatic Differentiation: the core technique of physics based machine learning.

1. The AD technique is not new; it has existed for several decades and many software exists.

2. The advent of deep learning drives the development of robust, scalable and flexible AD software that leverages the high performance computing environment.

3. As deep learning techniques continue to grow, crafting the tool to incorporate machine learning and AD techniques for inverse modeling is beneficial in scientific computing.

4. However, AD is not a panacea. Many scientific computing algorithms cannot be directly expressed by composition of differentiable operators.
ADCME is the materialization of the physics based machine learning concept.

ADCME allows users to use high performance and mathematical friendly programming language Julia to implement numerical schemes, and obtain the comprehensive automatic differentiation functionality, heterogeneous computing capability, parallelism and scalability provided by the TensorFlow backend.

https://github.com/kailaix/ADCME.jl
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