ADCME: Automatic Differentiation Library for Computational and Mathematical Engineering

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

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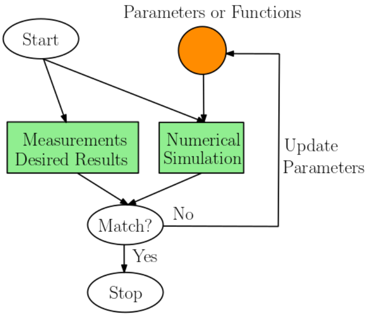
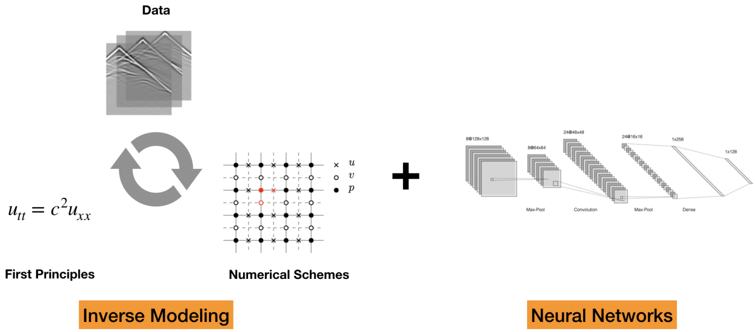
Inverse Modeling

- **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.



Physics Based Machine Learning

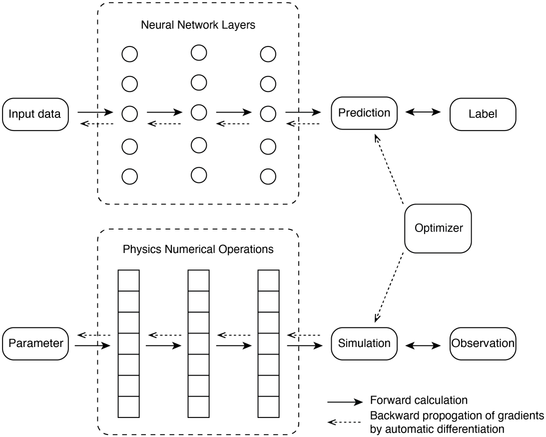
- Traditional inverse modeling methods utilize efficient numerical schemes and incorporate physical knowledge (first principles); deep learning learns statistical relations from large amounts of training data.
- We combine the best of the two worlds and invent **physics based machine learning**.



Automatic Differentiation

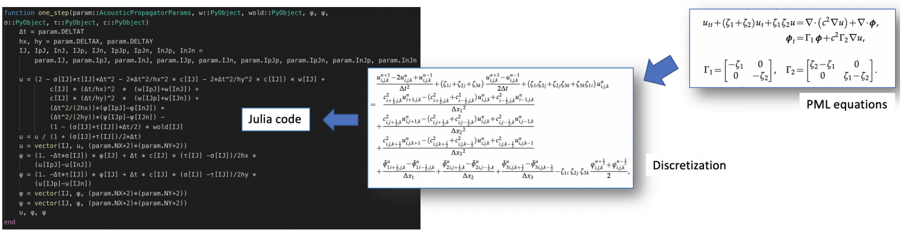
- Deep learning and inverse modeling have the same computational model but are disguised under different terminologies.

Back-propagation = Automatic Differentiation = Discrete Adjoint State Method



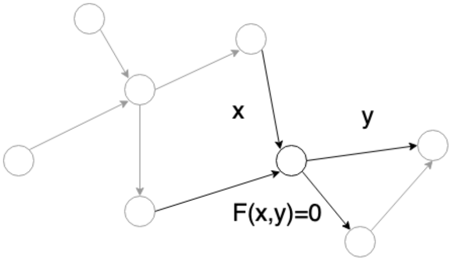
AD Implementation in ADCME

- ADCME allows users to use high level script language Julia to implement numerical simulation codes, but obtain the powerful parallelism and scalability provided by TensorFlow and Julia itself.
- Gradients are computed automatically.



Challenges in AD

- ADCME aims to solve the nonlinear implicit operator case via custom operators.
- Another ongoing effort is automatic calculation of Jacobian (`IGACS.jl`).



Linear/Nonlinear	Explicit/Implicit	Expression
Linear	Explicit	$y = Ax$
Linear	Implicit	$Ax = y$
Nonlinear	Explicit	$y = F(x)$
Nonlinear	**Implicit**	$F(x, y) = 0$

ADCME Solutions

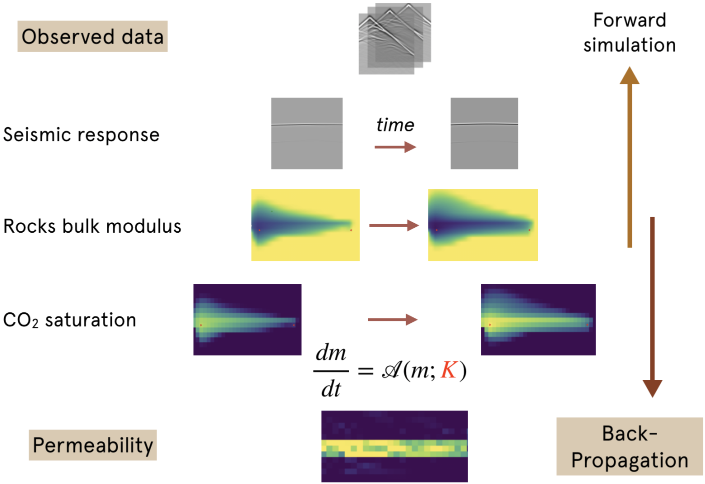
- Most inverse modeling problems can be classified into 4 categories. For example, the PDE for describing physics is

$$\nabla \cdot (X \nabla u) = 0 \quad \mathcal{BC}(u) = 0 \tag{1}$$

We observe some quantities depending on the solution u and want to estimate X.

Expression	Description	ADCME Solution	Note
$\nabla \cdot (c \nabla u) = 0$	Parameter Inverse Problem	Discrete Adjoint State Method	Direct optimize the constant c
$\nabla \cdot (f(x) \nabla u) = 0$	Functional Inverse Problem	Neural Network Functional Approximator	$f(x) \approx f_\theta(x)$
$\nabla \cdot (f(u) \nabla u) = 0$	Relation Inverse Problem	Deep Learning for Indirect Data	$f(u) \approx f_\theta(u)$
$\nabla \cdot (\varpi \nabla u) = 0$	Stochastic Inverse Problem	Adversarial Numerical Analysis	Generative Neural Nets for ϖ (unknown random processes)

Parameter Inverse Problem: Learning Hidden Geophysical Processes



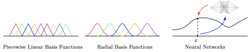
Functional Inverse Problem: Calibrating Lévy Processes

$$\phi(\boldsymbol{\xi}) = \mathbb{E}[e^{\mathrm{i}\langle \boldsymbol{\xi}, \mathbf{X}_t\rangle}] =$$

$$\exp\left[t\left(\mathrm{i}\langle \mathbf{b}, \boldsymbol{\xi}\rangle - \frac{1}{2}\langle \boldsymbol{\xi}, \mathbf{A}\boldsymbol{\xi}\rangle + \int_{\mathbb{R}^d}\left(e^{\mathrm{i}\langle \boldsymbol{\xi}, \mathbf{x}\rangle} - 1 - \mathrm{i}\langle \boldsymbol{\xi}, \mathbf{x}\rangle \mathbf{1}_{\|\mathbf{x}\|\le 1}\right)\nu(d\mathbf{x})\right)\right]$$

Model

$$\nu(\mathbf{x}) \approx \nu_{\boldsymbol{\theta}}(\mathbf{x})$$

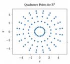


$$\downarrow$$

$$\phi(\boldsymbol{\xi}) \approx \phi_{\boldsymbol{\theta}}(\boldsymbol{\xi}) := \exp\left[\Delta t \sum_{i=1}^{n_q}\left(e^{\mathrm{i}\langle \boldsymbol{\xi}, \mathbf{x}_i\rangle} - 1 - \mathrm{i}\langle \boldsymbol{\xi}, \mathbf{x}_i\rangle \mathbf{1}_{\|\mathbf{x}_i\|\le 1}\right)\nu_{\boldsymbol{\theta}}(\mathbf{x}_i) w_i\right]$$

$$\downarrow$$

$$\boxed{\min_{\boldsymbol{\theta}} \frac{1}{m}\sum_{i=1}^{m}\|\hat{\phi}_n(\boldsymbol{\xi}_i) - \phi_{\boldsymbol{\theta}}(\boldsymbol{\xi}_i)\|^2}$$



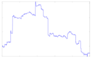
$$\uparrow$$

Data

$$\hat{\phi}_n(\boldsymbol{\xi}) := \frac{1}{n}\sum_{i=1}^{n}\exp(\mathrm{i}\langle \boldsymbol{\xi}, \mathbf{X}_{i\Delta t} - \mathbf{X}_{(i-1)\Delta t}\rangle),\ \boldsymbol{\xi} \in \mathbb{R}^d$$

$$\uparrow$$

$$\{\mathbf{X}_{i\Delta t}\}_i$$



Relation Inverse Problem: Learning Constitutive Relations

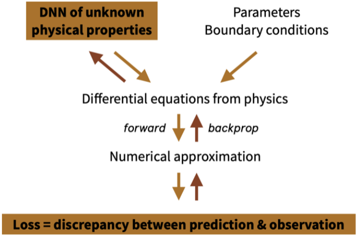
- Equilibrium equation

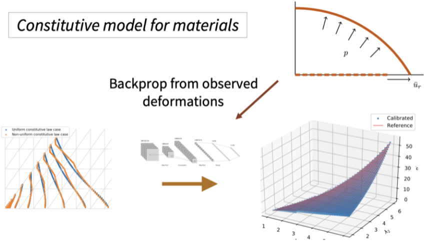
$$\mathcal{P}(u(\mathbf{x}), \mathcal{M}(u(\mathbf{x}), \dot{u}(\mathbf{x}), \mathbf{x})) = \mathcal{F}(u(\mathbf{x}), \mathbf{x}, p)$$

- Neural Network Approximation:

$$\mathcal{M}_\theta(\mathbf{u}) \approx \mathcal{M}(u(\mathbf{x}), \dot{u}(\mathbf{x}), \mathbf{x})$$

$$\boxed{\min_\theta \|\mathcal{P}(\mathbf{u}, \mathcal{M}_\theta(\mathbf{u})) - \mathcal{F}(\mathbf{u}, \mathbf{x}, p)\|_2^2}$$

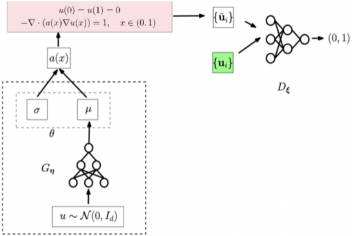


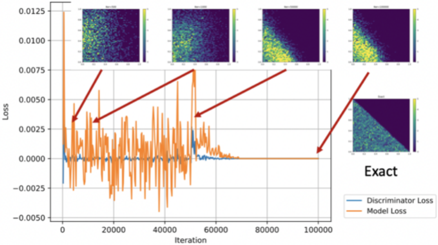


Probability Inverse Problem: Adversarial Numerical Analysis

$$\begin{cases} -\nabla \cdot (a(x)\nabla u(x)) = 1 & x \in (0,1) \\ u(0) = u(1) = 0 & \text{otherwise} \end{cases}$$

$$a(x) = 1 - 0.9 \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$





A Cool Application: `ADSeismic.jl` (Coming soon)

- An Open Source High Performance Package for General Seismic Inversion Problems
- Problems include:
    - Full waveform inversion (FWI);
    - Rupture inversion;
    - Source-time inversion.
- Features:
    - (Multi-)GPU support;
    - Easy-to-use;
    - Easily extendable.