Algorithmic differentiation for mixed FEniCS-TensorFlow models

Simon W. Funke, Sebastian Mitusch

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Deep Learning:
A Critical Appraisal

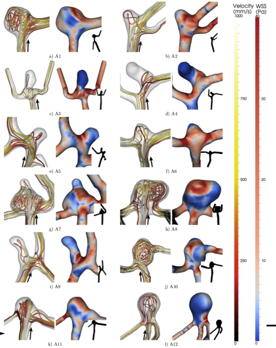
Gary Marcus, 2018

3.6. Deep learning thus far has not been well integrated with prior knowledge

“[...] researchers in deep learning appear to have a very strong bias against including prior knowledge even when (as seen in the case of physics) that prior knowledge is well known.”

Can we improve clinical decisions of aneurysm removals?

Physical simulations



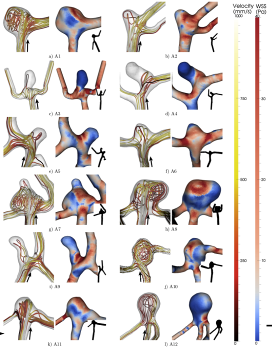
K.A.Maradal et al

Patient specific data
Aneurysm geometry,
patient age, diet,
genetic properties

Clinical decision

Can we improve clinical decisions of aneurysm removals?

Physical simulations



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Patient specific data
Aneurysm geometry,
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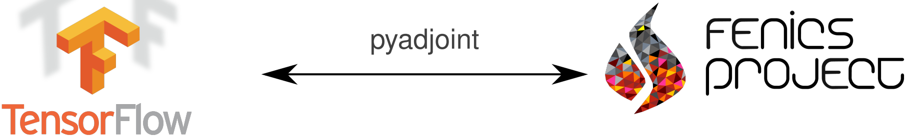
Clinical decision

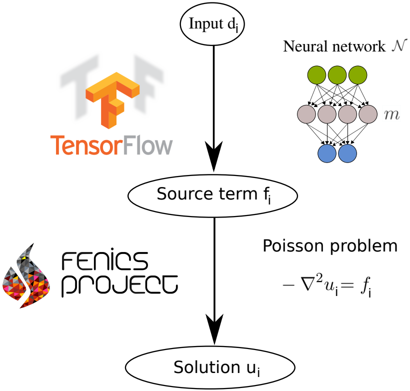
Patient specific data → PDE Model → ML Model → **Clinical decision**

The software landscape is currently divided



We consider a minimal mixed PDE-NN problem

Model



Training

Given:

- training inputs $d_1, ..., d_N$,
- training outputs $y_1, ..., y_N$,

Solve:

$$\min_m \sum_{i=1}^{N} \|u_i - y_i\|$$

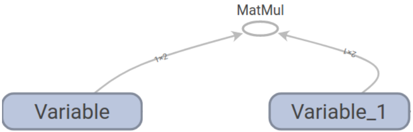
subject to:

$$f_i = \mathcal{N}(d_i; m) \quad \forall i$$
$$-\nabla^2 u_i = f_i \quad \forall i$$

TensorFlow is a generic tensor computation platform

- TensorFlow creates a computation graph of tensor operations.
- Tensor models use lazy evaluation to optimization for CPUs/GPUs computations.

```
import tensorflow as tf

t1 = tf.Variable([[3., 3.]])
t2 = tf.Variable([[2.],[2.]])
product = tf.matmul(t1, t2)

with tf.Session() as sess:
    result = sess.run(product)
    print(result)
```



Implementation of a neural network with one hidden layer

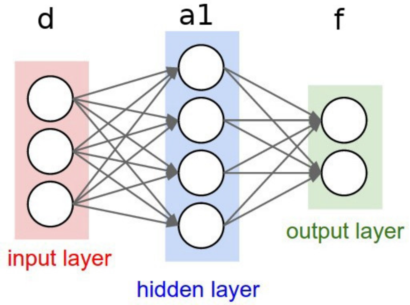


Image: cs231n.github.io

- $b1, b2, W1, W2$ are the training parameters.
- We use $\tanh$ as activation function and identity for the output layer.

```
d = tf.placeholder(...)

W1 = tf.Variable(...)
b1 = tf.Variable(...)
W2 = tf.Variable(...)
b2 = tf.Variable(...)

a1 = tf.matmul(d, W1) + b1
z1 = tf.tanh(a1)
f = tf.matmul(z1, W2) + b2
```

The FEniCS models is added as a custom TensorFlow operation

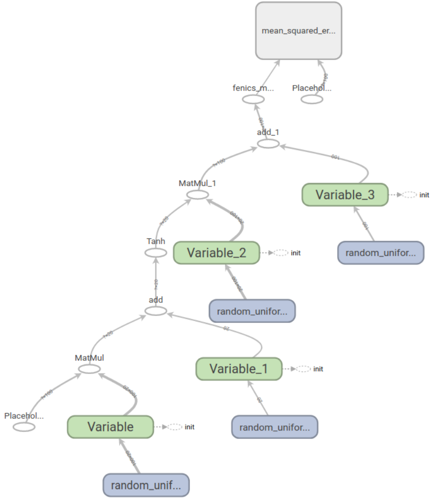
- We implemented convenience functions[1] in pyadjoint to
  - convert FEniCS and TensorFlow data structure.
  - register function as a TensorFlow operation.
- Lazy evaluation of FEniCS model is achieved by pass-as-function.

```
from fenics import *
from pyadjoint import *

def poisson(f):
    ...
    f = tf_to_fenics(f, V)
    solve(a==f*v*dx, u)
    return fenics_to_tf(u)

y=register_tf_function(poisson)(f)
```

[1] still under active development

Define loss function and optimiser. Are we done?

```
loss = tf.losses.mean_squared_error(labels=y_, predictions=y)
optimizer = tf.train.GradientDescentOptimizer()
optimizer.minimize(loss)
```



TensorFlow computation graph

... No! TensorFlow uses back-propagation to evaluate gradients during model training

- Gradients of TensorFlow operations are automatically derived.
- Custom operations require manual gradient implementation.
  A custom function

$$\begin{aligned} x &\to J(x) \\ \mathbb{R}^m &\to \mathbb{R}^n \end{aligned}$$

  needs implementing

$$\begin{aligned} y &\to y^T J'(x) \\ \mathbb{R}^n &\to \mathbb{R}^m \end{aligned}$$

FEniCS models require an adjoint solve to compute the gradient

- We have $J(u, x)$, where u is the solution of a PDE $F(u, x) = 0$.
- In this case, we need to compute

$$y \to y^T \left(\frac{\partial J}{\partial u} \frac{\mathrm{d}u}{\mathrm{d}x} + \frac{\partial J}{\partial x} \right)$$

- This is computed efficiently by solving the adjoint problem of

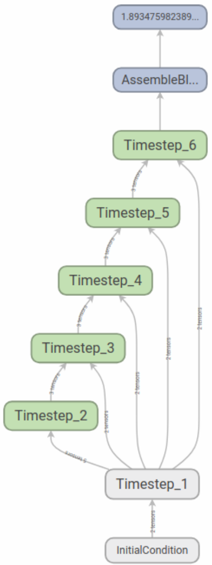
$$y^T J(u, x)$$

subject to

$$F(u, x) = 0$$

We rely on pyadjoint to automate the adjoint of FEniCS models

- pyadjoint creates a computation graph of the FEniCS model
- On TensorFlow's request, pyadjoint defines the auxiliary functional and solves the adjoint problem.



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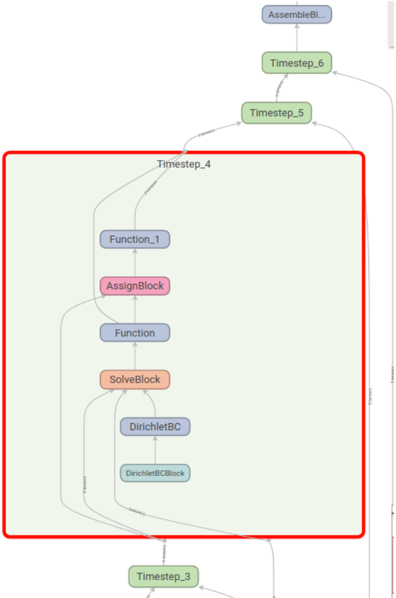


We obtain correct gradients for the minimal neural network Poisson problem

Setup:

- Input: d
- Single layer neural network $f = \mathcal{N}(d, b_1, W_1, b_2, W_2)$
- PDE: $-\Delta u = f$
- 20 nodes in the hidden layer, random training set of size $N = 50$

Results:

2nd order Taylor test results with respect to $b2$

Perturbation size	convergence order
1	-
$1/2$	2.00
$1/4$	2.00
$1/8$	2.00

We also obtain correct gradients with respect to PDE coefficients

Setup:

- Input: f
- PDE: $-\lambda \Delta u = f$
- Single layer neural network $y = \mathcal{N}(u, b_1, W_1, b_2, W_2)$.
- 20 nodes in the hidden layer, random training set of size $N = 50$.

Results:

2nd order Taylor test results with respect to λ

Perturbation size	Convergence order
1	-
$1/2$	2.00
$1/4$	2.00
$1/8$	2.00

Optimisation problem

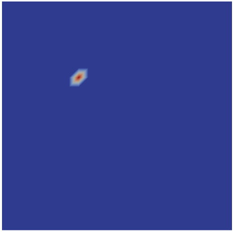
Ground truth model:

- Input: f
- PDE: $u - \lambda \Delta u = f$
- Output: Point evaluation $y = u(x)$

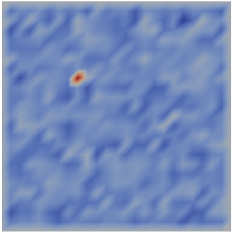
Setup:

- Input: f
- PDE: $u - \lambda \Delta u = f$
- 0-level "neural network": $y = \mathcal{N}(u, b1)$
- Training data: 100 data points generated from random source terms f
- Optimiser: RMSProp, 500 iterations

Results:



True evaluation function



Optimised neural network weights

Thank you for listening!

Follow us on bitbucket.org/dolfin-adjoint/pyadjoint