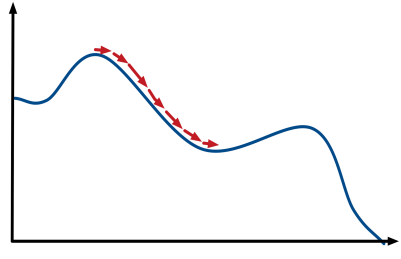

# Fitting IceCube Ice Model Parameters with Gradient Descent

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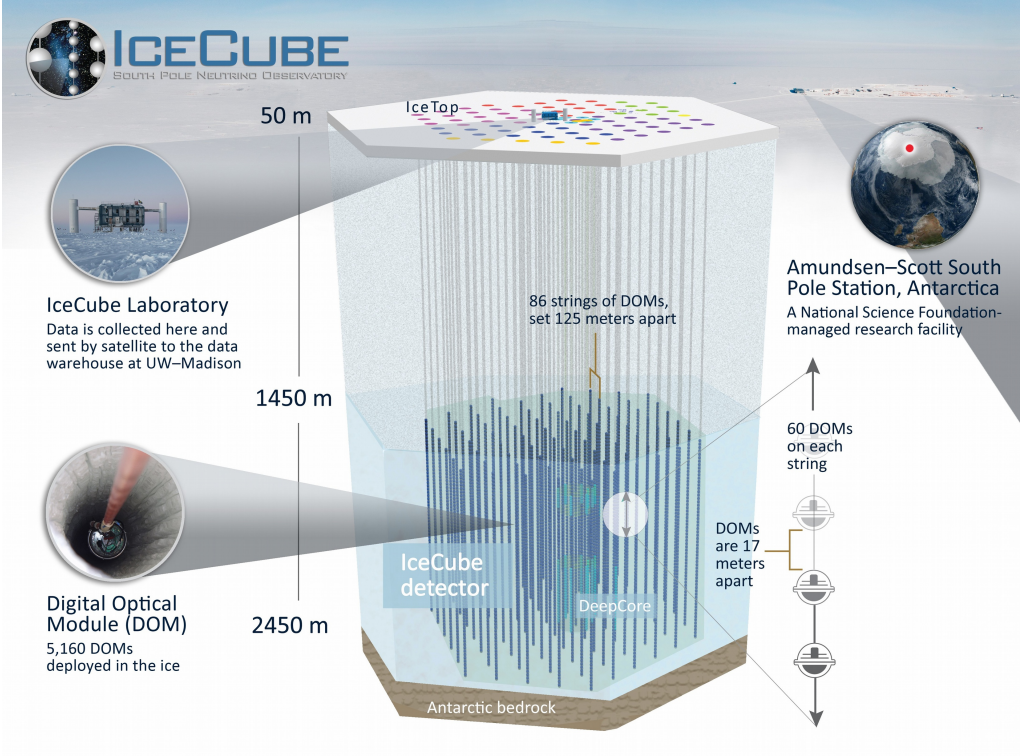
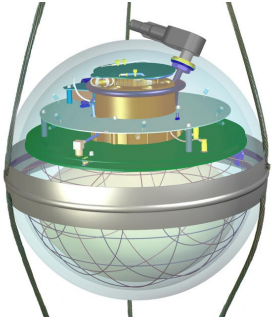
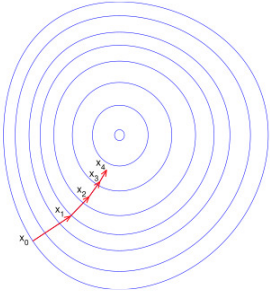

IceCube
South Pole Neutrino Observatory
50 m
IceTop
IceCube Laboratory
Data is collected here and sent by satellite to the data warehouse at UW–Madison
86 strings of DOMs, set 125 meters apart
Amundsen–Scott South Pole Station, Antarctica
A National Science Foundation-managed research facility
1450 m
60 DOMs on each string
DOMs are 17 meters apart
IceCube detector
DeepCore
Digital Optical Module (DOM)
5,160 DOMs deployed in the ice
2450 m
Antarctic bedrock

## Introduction



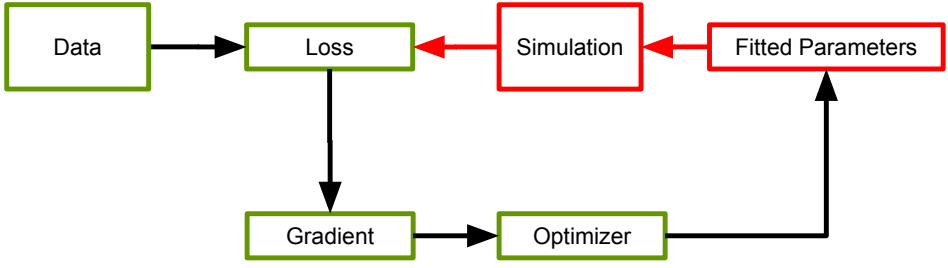
- IceCube detects neutrinos by measuring the Cherenkov light emitted by secondary particles
- For that we need precise simulations of photon propagation within the ice
- For modeling the ice we divide it into layers in $z$ direction
- There are global ice model parameters and parameters for each layer, mainly scattering and absorption coefficients
- There is a flasher board on each DOM which we use as light sources for callibration

## Motivation



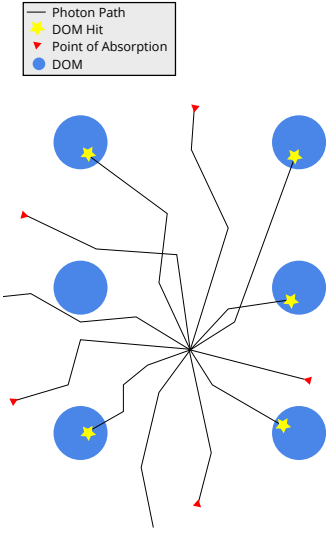

- Fitting ice parameters by performing iterative grid searches is extremely complex and time-consuming
- We want to compute gradients of the likelihood, to be able to perform gradient descent instead of grid searches
- This might reduce the cost and improve scalability
- For now we focused on bulk ice absorption coefficients
- We should at least be able to verify the current best fit using this independent method

## General Idea




**Challenge:** Making the red part differentiable.

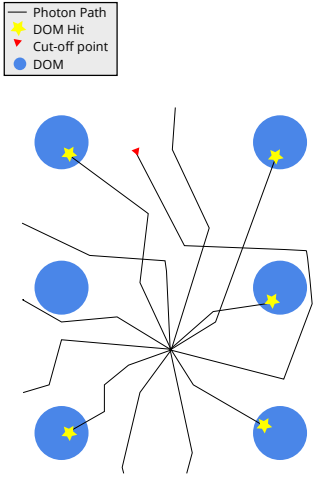
## Photon Propagation Simulation - Before




1. Initialize photons
2. While not hit or absorbed
   - 2.1 Propagate photon
     - Hit? Stop propagation at DOM contact point
     - Absorbed? Stop propagation at point of absorption
     - Otherwise propagate to next scattering point
   - 2.2 Scatter photon, if not hit or absorbed
3. Output: DOM responses

See pseudo code on backup-slide 23

## Photon Propagation Simulation - Modified to Allow Differentiation




1. Initialize photons
2. While not hit or cut-off reached
   - 2.1 Propagate photon
     - Hit? Stop propagation at DOM contact point
     - Cut-off reached? Stop propagation
     - Otherwise propagate to next scattering point
     - **Log traveled distance in each layer**
   - 2.2 Scatter photon, if not hit or cut-off
3. Intermediate output for each hit: The DOM that was hit and the traveled distance in each layer

Cut-off based on total travel distance and ignore all photons, that were cut-off.

## Calculate DOM Response from Intermediate Result

Input: Photon travel distances $D_j$ for each layer $j$ and which DOM was hit for each Photon, that hit a DOM.

Calculate the probability for each photon to reach the DOM, after propagation:

$$\begin{aligned} p_{\text{Hit}} = 1 - p_{\text{Absorbed}} &= \exp\left(-\int_0^D a(x)\mathrm{d}x\right) \\ &\overset{\text{Layer}}{=} \exp\left(-\sum_{j=1}^{N_{\text{Layer}}} a_j D_j\right) \end{aligned} \tag{1}$$

where $a_j$ is the absorption coefficient of the $j$-th layer.

Output: Summed hit probabilities of all photons for each DOM

$$s_i = \sum_{j=1}^{N_{\text{Hits},i}} p_{\text{Hit},ij} \tag{2}$$

## Getting the Gradient

The loss $F$ we are trying to minimize is the negative logarithm of the likelihood ratio

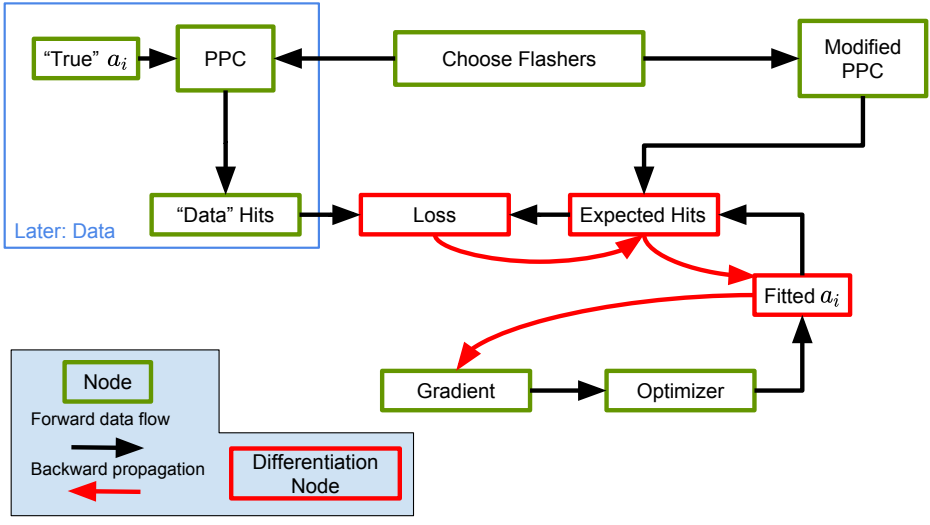
$$-F = \log \mathcal{L}_{\text{Ratio}} \,. \tag{3}$$

We now have a direct chain between a suitable loss function $F$ and absorption coefficients whitout any control statements, which we can use to compute the gradient

$$\nabla_{\vec{a}} F = \cdots \tag{4}$$

by using TensorFlow's automatic differentiation (backpropagation). We could also define the gradient by hand, which would be simple but tedious.

## Fitting Algorithm



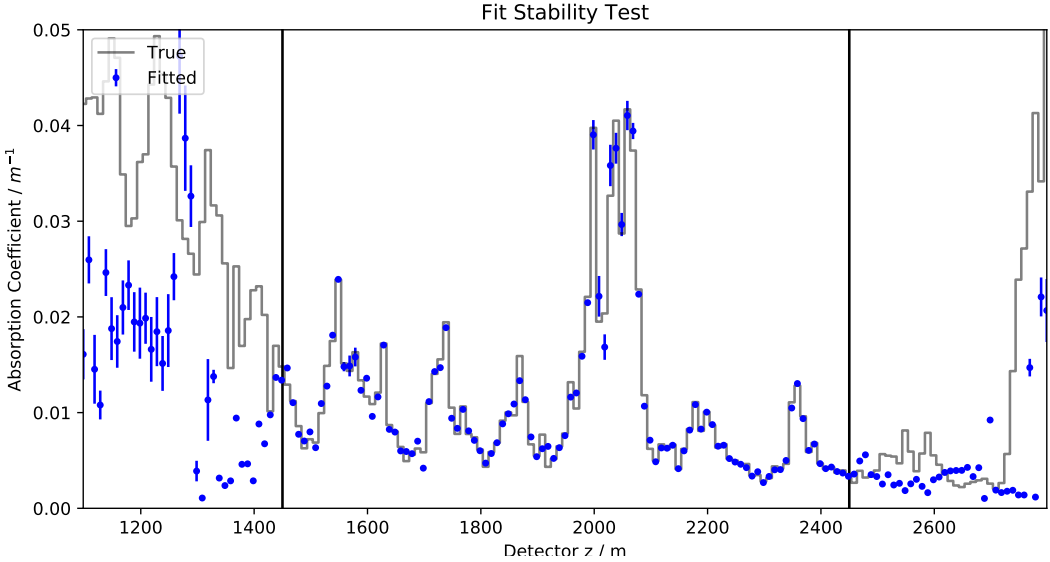
## Videos of the Learning Progress

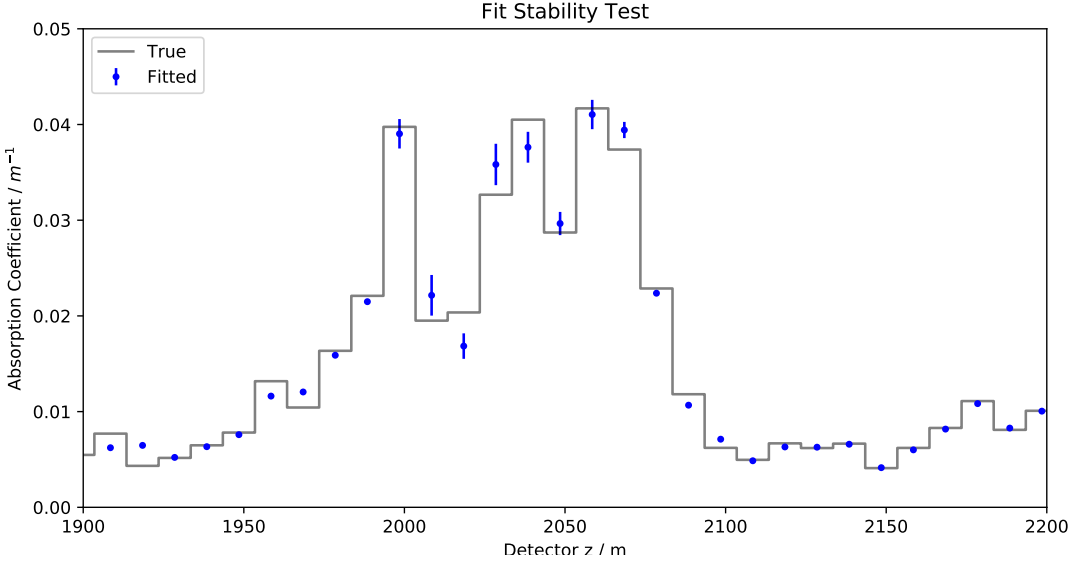
Hyperlinks to videos:

- Initial coefficients all set to $0.008\,\mathrm{m}^{-1}$
  - 10 times faster
- Initial coefficiens sampled uniformly between $0.005\,\mathrm{m}^{-1}$ and $0.03\,\mathrm{m}^{-1}$
  - 10 times faster

## Fit Stability Test

- Idea: Fit multiple times with random initial values to check for stability
- 8 runs with initial coefficients sampled uniformly between $0.005\,\mathrm{m}^{-1}$ and $0.03\,\mathrm{m}^{-1}$
- The following plots show the mean and standard deviation of the mean of those 8 fit results


Fit Stability Test
True
Fitted
Absorption Coefficient / $m^{-1}$
Detector z / m
0.00
0.01
0.02
0.03
0.04
0.05
1200
1400
1600
1800
2000
2200
2400
2600


Fit Stability Test
True
Fitted
Absorption Coefficient / $m^{-1}$
Detector z / m
0.00
0.01
0.02
0.03
0.04
0.05
1900
1950
2000
2050
2100
2150
2200

## Conclusion and Outlook

Seems to be working! We should at least be able to verify the current fit with this independent approach.

Problems:

- Uncertainty on LED light output for real data
- Performance: Copying stuff around GPU and CPU memory. Need for general optimization

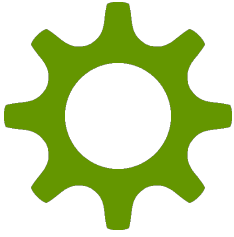
Ideas:

- Scattering: Many possible approaches
  - Assuming a strong correlation between absorption and scattering
  - Hybrid between grid search and gradient descent approach
  - Estimating the gradient for scattering coefficients, e.g. by resampling the arrival time for each photon
- Anisotropy: Tessellated sphere idea proposed by Martin Rongen
- Possibly do hardware simulation
- Use timing information

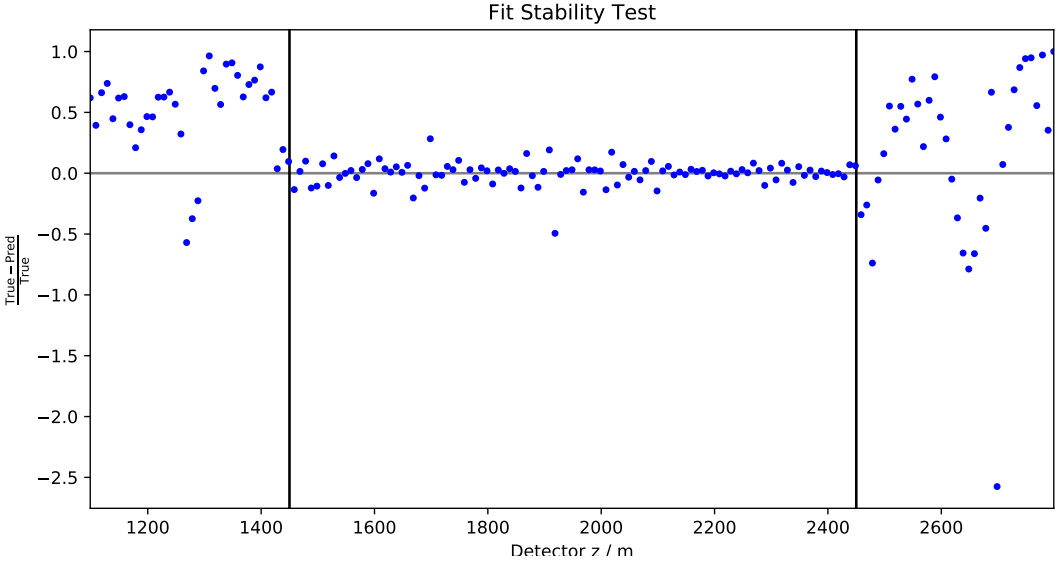
Next? Moving on towards using real data and incorporate scattering.

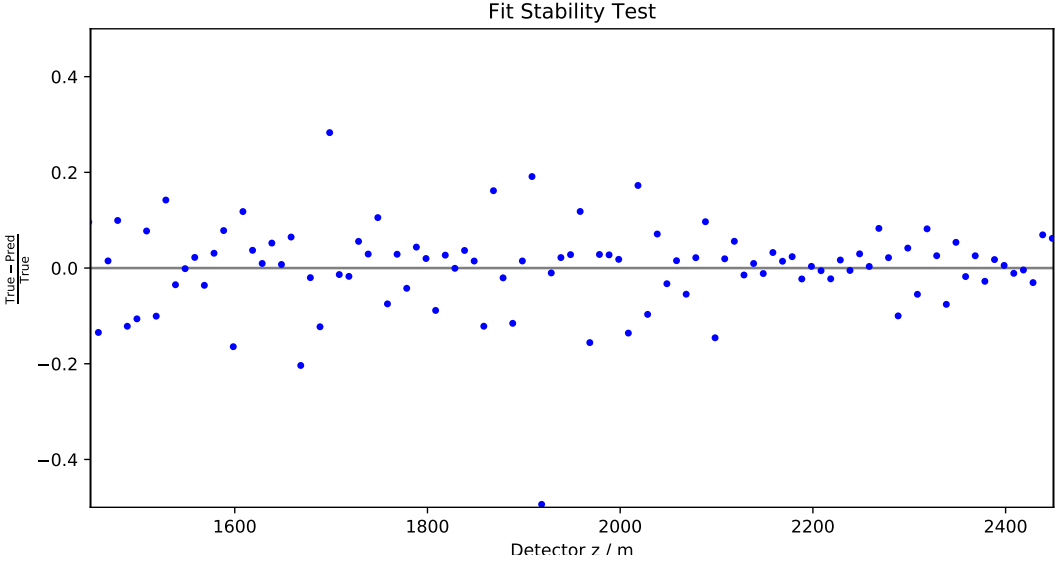
# Backup

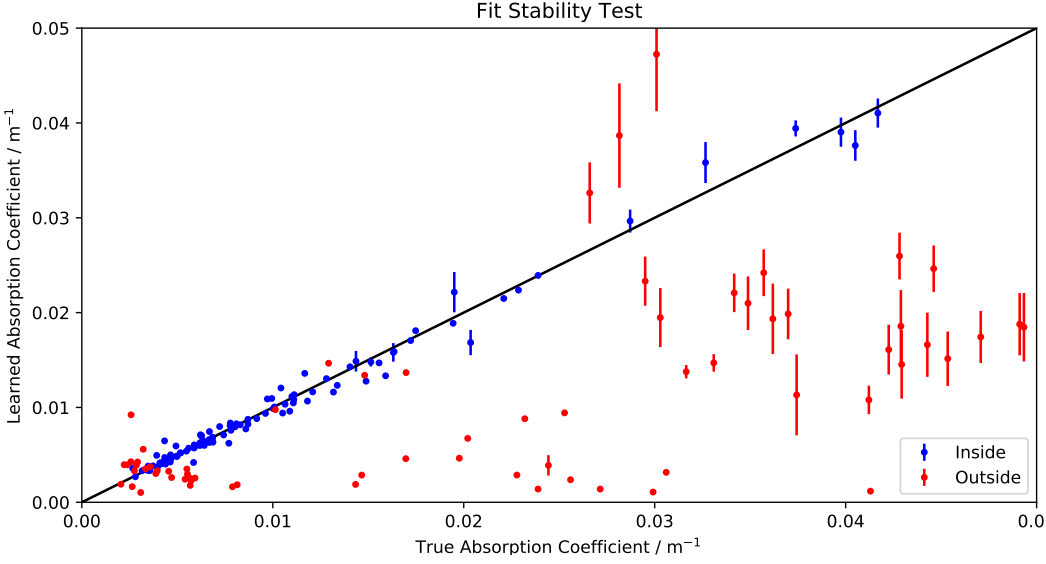
## Test Setup



- Two seperate PPC executables, one without absorption and the other one unmodified to generate fake data to fit to
- Using the current 3.2 best fit values to generate the fake data
- The scattering coefficients are fixed to the “True” values for the fit
- Anisotropy is disabled
- DOM-Oversizing of 15, should be fine since we don’t use arrival time information yet
- All photons have the same wavelength of $400\,\mathrm{nm}$ (PPC WFLA=400)
- Flashing all DOMs on string 36 (inside deep core) to generate batches
- Emitting $1.5 \cdot 10^7$ photons for each batch
- All following fits were done on the same fake dataset which consists of 347 batches


Fit Stability Test
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
True − Pred / True
1200
1400
1600
1800
2000
2200
2400
2600
Detector z / m


Fit Stability Test
0.4
0.2
0.0
−0.2
−0.4
True − Pred / True
1600
1800
2000
2200
2400
Detector z / m


Fit Stability Test
Learned Absorption Coefficient / m$^{-1}$
True Absorption Coefficient / m$^{-1}$
0.00
0.01
0.02
0.03
0.04
0.05
Inside
Outside

## The Problem with Differntiating the Propagation Loop

- Automatic differentiation works great for arbitrarily complex programs and can deal with control statements.
- There is one caveat: Those control statements must not depend on the target parameters of the differentiation.
  - In that case the structure of the program changes depending on the target parameter, information about other branches of the program is not included in a mathematical derivative of the one branch that was executed.
  - It can still work in some cases (e.g. our first results) but generally there is no guarantee for the gradient to point in the right direction.

## The Problem - Super Simple Example

Consider the following program:

```
def y(x):
  if x == 2:
    return 4
  else:
    return 2*x
```

- In case of $x \neq 2$ automatic differentiation will provide the correct derivative of $\frac{\partial y}{\partial x} = 2$. In case of $x = 2$ the derivative is $0$, but we need it to be $2$ in that case as well.
- Automatic differentiation simply evaluates the chain rule along the executed branch of the program. This is only fine as long as the branching does not depend on target parameters.
- In this case the problem could be easily resolved by defining the gradient manually or rewriting the program.

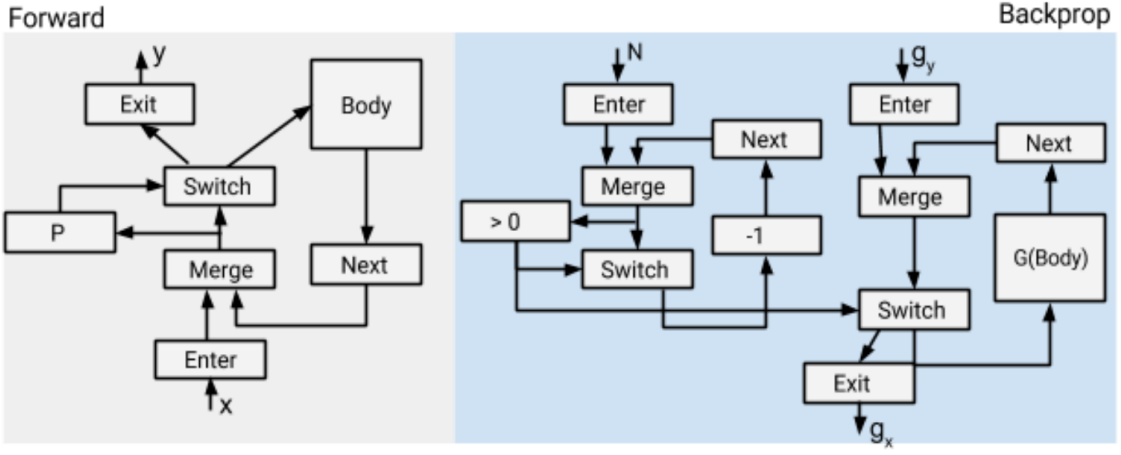
## The Problem - Our Case

Our case looks like this (simplified pseudo code):

```
def simulate(photon, l_abs, l_scat):
  d_abs = sample_absorption(l_abs)
  while d_abs > 0 and not hit:
    d_scat = sample_scattering(l_scat)
    hit = check_for_hits(photon, d_scat)
    if hit:
      propagate_to_hit(photon)
    else:
      if d_abs - d_scat > 0:
        propagate(photon, d_scat)
        scatter(photon)
        d_abs -= d_scat
      else:
        propagate(photon, d_abs)
        d_abs = 0
```

- During forward propagation Tensorflow counts the number of loop iterations. When backpropagating the number of loop iterations is therefore a constant.
- **This means the gradient “does not know” that changing a scattering or absorption length a little bit would lead to one more/less scattering process, even though the derivative of a single scattering process is correct.**
- More on this is explained in the reference given on slide 24 and in a demonstration we wrote.

## Tensorflow While Loop - Problem

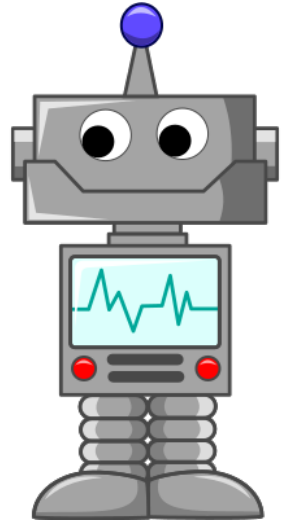



Source: http://download.tensorflow.org/paper/white_paper_tf_control_flow_implementation_2017_11_1.pdf

Problem: $N$ is a constant during backprop. $P$ must not depend on target variables, but it does in our case.

## Automatic Differentiation - Introduction

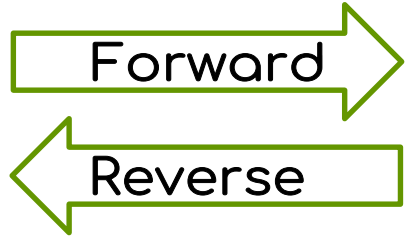
- Set of techniques to evaluate derivatives of functions given by computer programs
- Every computer program can be broken down to a number of basic mathematical operations
- If the derivative of those operations is known, we can use the chain rule to get the derivative of the entire program, which is the basic idea of AD
- It is not symbolic nor numerical differentiation (often confused)
- Can be applied to arbitrarily complex functions, like simulations



## Automatic Differentiation - Forward and Reverse Mode

- Two possible approaches: Forward and reverse mode
- Essentially the direction in which we apply the chain rule
- Reverse mode is divided into two phases: **forward pass** and **backward pass**
- Backward pass is often called backpropagation in machine learning
- We use TensorFlow, which uses reverse mode AD

$$\frac{\partial f_n}{\partial x} = \frac{\partial f_0}{\partial x}\frac{\partial f_1}{\partial f_0}\cdots\frac{\partial f_n}{\partial f_{n-1}}$$

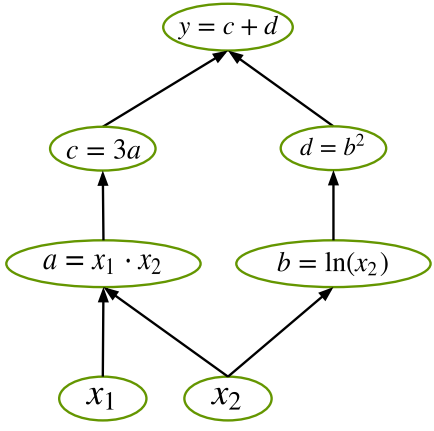


## Automatic Differentiation Example - Computational Graph

Let's look at a simple example

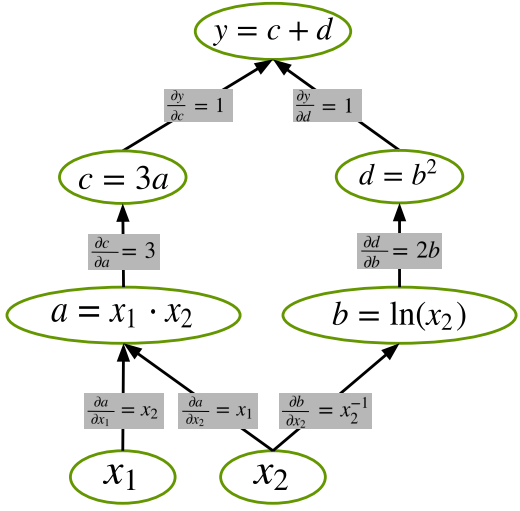
$$y = f(x_1, x_2) = 3x_1x_2 + \ln^2(x_2) \tag{5}$$

The **computational graph** looks like this



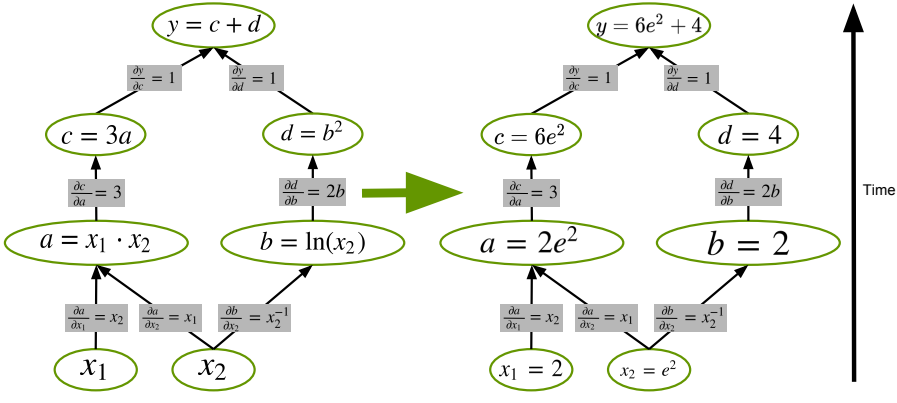
## Automatic Differentiation Example - Node Derivatives

We know the derivatives of every node:



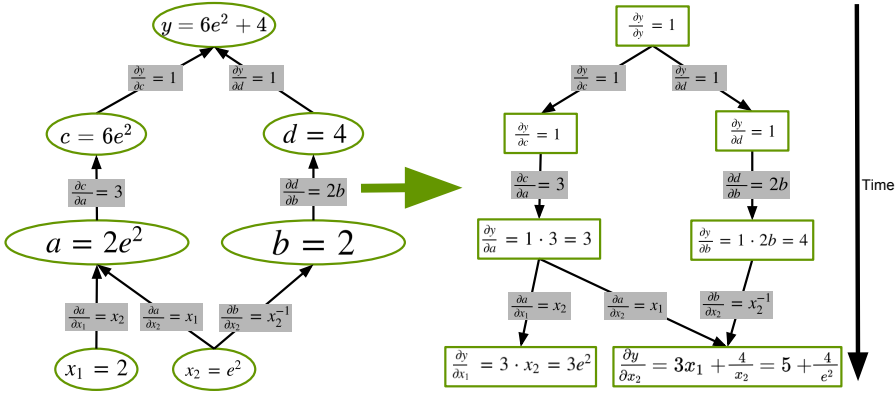
## Automatic Differentiation Example - Forward Pass

Let's evaluate the gradient for $x_1 = 2$ and $x_2 = e^2$ with reverse mode AD. First we perform the **forward pass** and save all the intermediate results:



## Automatic Differentiation Example - Backward Pass

To obtain the gradient $(\frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2})^\mathsf{T}$ we apply the chain rule by traversing the graph in reverse order:




As expected by doing this we evaluate chain rule terms like $\frac{\partial y}{\partial x_1} = \frac{\partial y}{\partial c}\frac{\partial c}{\partial a}\frac{\partial a}{\partial x_1}$ from outside to inside.