TensorFlow tutorial

Adam Elwood

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Introduction and outline

- This is a tutorial designed to give a very basic introduction to the main concepts behind TensorFlow, consisting of:
    - A very brief overview of neural networks from a TensorFlow standpoint
    - TensorFlow as a computational graph framework
    - How Automatic Differentiation works
    - A simple example of classifying two different Gaussians with a neural network
- Following this there is an exercise to practice writing your own simple network with TensorFlow in a HEP context
- Thanks to Stefan Wunsch who provided the inspiration and lots of material for this tutorial in the IML workshop in April
    - https://indico.cern.ch/event/668017/contributions/2947042/
    - https://github.com/stwunsch/iml_tensorflow_keras_workshop

Introduction to TensorFlow

- TensorFlow is a low-level implementation of operations needed to implement neural networks in multi-threaded CPU and multi GPU environments
- Differences with **PyTorch** (Facebook vs Google)
  - TensorFlow designed to use static graph definition, you have to build the graph then compile it before running
  - PyTorch allows the graph to be built and executed dynamically
  - TensorFlow is currently the most widely used but PyTorch is gaining popularity
  - Generally speaking: TensorFlow better for production code and PyTorch better for research
  - More info: https://towardsdatascience.com/pytorch-vs-tensorflow-spotting-the-difference-25c75777377b
  - **Disclaimer**: these frameworks are developing so quickly this information may not stay relevant
- **Keras** provides high-level convenience wrapper for backend libraries, predominantly TensorFlow, to implement neural network models
  - Will be covered in much more detail later

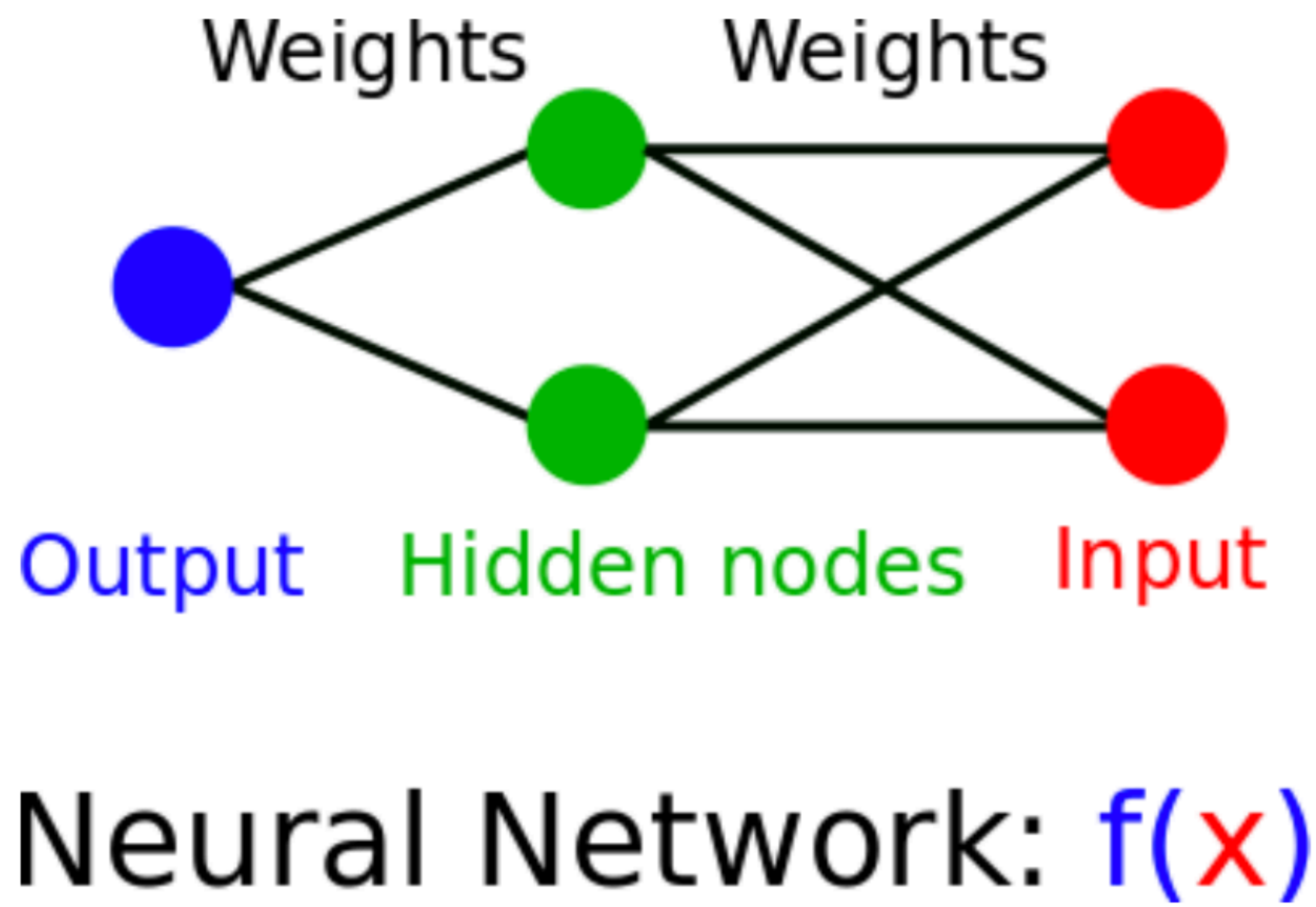
vs

Source for code

- Github repository containing the slides and examples:
  - https://github.com/aelwood/iml_tensorflow_keras_workshop
- Notebooks relevant to this tutorial in 'tensorflow' folder
- Setup instructions:

```
# get the repository
git clone https://github.com/aelwood/iml_tensorflow_keras_workshop.git
cd iml_tensorflow_keras_workshop

# install necessary software, this may be already available
# e.g. setup with conda
source init_virtualenv_conda.sh
#or pip (you can just select the modules you need from this file)
source init_virtualenv.sh

cd tensorflow
jupyter notebook gaussian.ipynb #for example
```

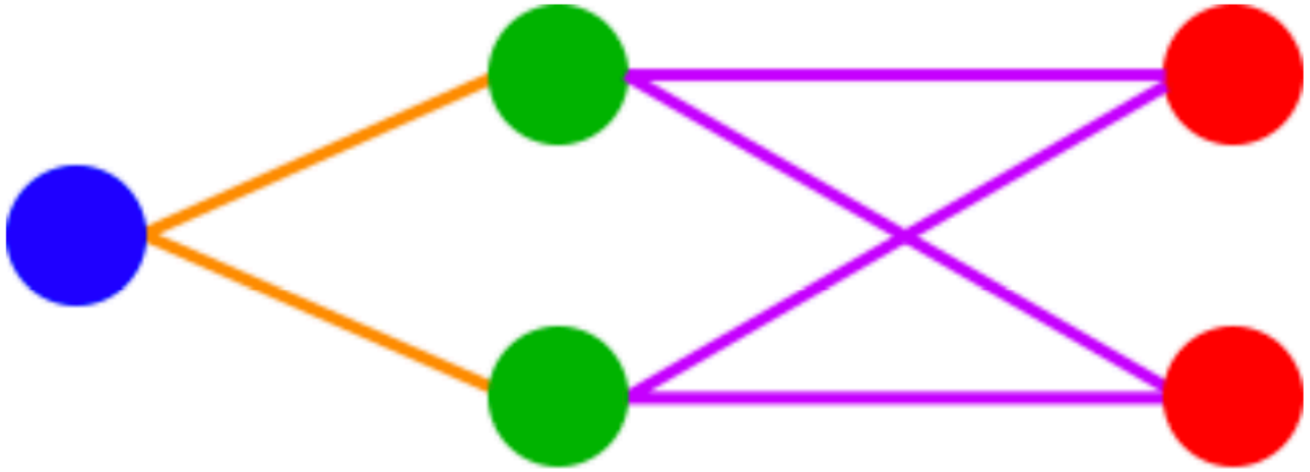
A simple neural network



- **Important:** A neural network is only a mathematical function. No magic involved!
- **Training:** Finding the best function for a given task, e.g., separation of signal and background.

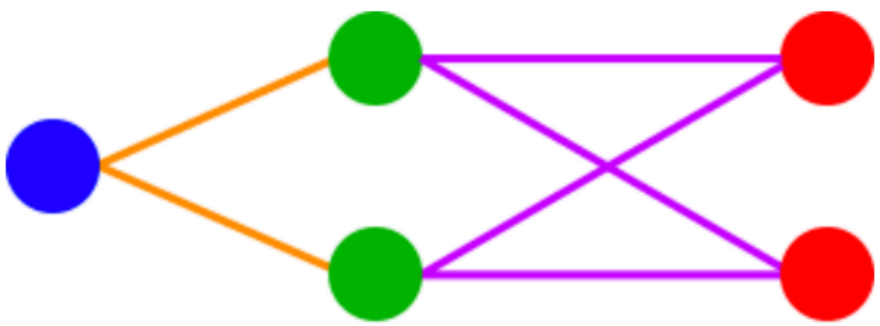
Mathematical representation

- **Why do we need to know this?**
  $\rightarrow$ TensorFlow implements these mathematical operations explicitely.
  $\rightarrow$ Basic knowledge to understand Keras' high-level layers.



$$f_{NN} = \sigma(b_2 + W_2\sigma(b_1 + W_1 x))$$

Mathematical representation (2)



$f_{NN} = \sigma(b_2 + W_2\sigma(b_1 + W_1 x))$

$$\text{Input} : x = \begin{bmatrix} x_{1,1} \\ x_{2,1} \end{bmatrix}$$

$$\text{Weight} : W_1 = \begin{bmatrix} W_{1,1} & W_{1,2} \\ W_{2,1} & W_{2,2} \end{bmatrix}$$

$$\text{Bias} : b_1 = \begin{bmatrix} b_{1,1} \\ b_{2,1} \end{bmatrix}$$

$$\text{Activation} : \sigma(x) = \tanh(x) \quad \text{(as example)}$$

Activation is applied elementwise!

The "simple" neural network written as full equation:

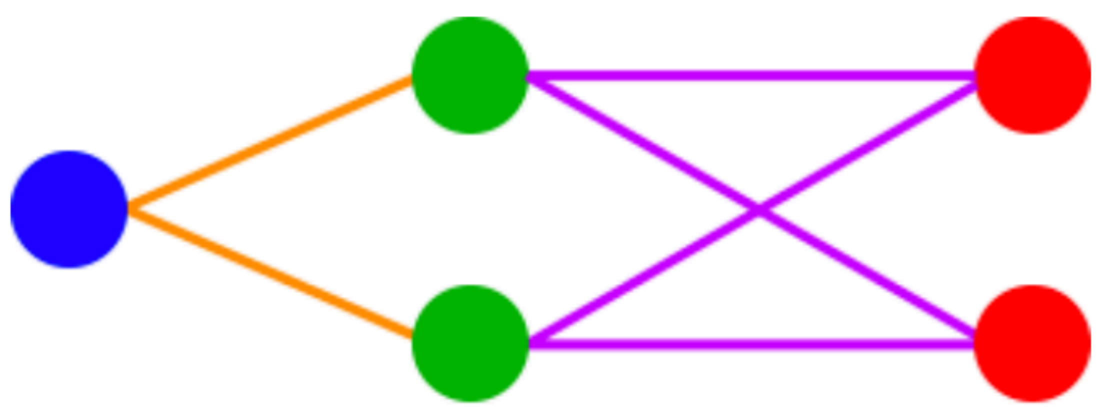
$$f_{\mathrm{NN}} = \sigma_2\left(\begin{bmatrix} b^2_{1,1} \end{bmatrix} + \begin{bmatrix} W^2_{1,1} & W^2_{1,2} \end{bmatrix} \sigma_1\left(\begin{bmatrix} b^1_{1,1} \\ b^1_{2,1} \end{bmatrix} + \begin{bmatrix} W^1_{1,1} & W^1_{1,2} \\ W^1_{2,1} & W^1_{2,2} \end{bmatrix} \begin{bmatrix} x_{1,1} \\ x_{2,1} \end{bmatrix}\right)\right)$$

S.Wunsch: https://indico.cern.ch/event/668017/contributions/2947042/

What is TensorFlow?

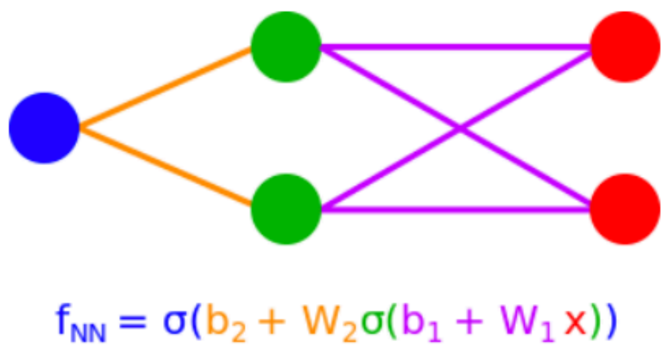
TensorFlow *is an open source software library for* ***numerical computation using data flow graphs****. Nodes in the graph represent mathematical operations, while the graph edges represent the multidimensional data arrays (tensors) communicated between them.*

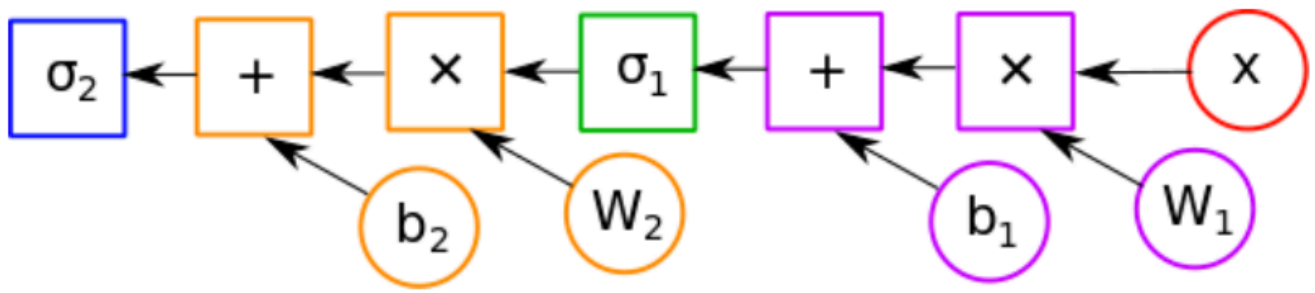
- **In first place:** TensorFlow is not about neural networks.
- But it is a **perfect match** to implement neural networks efficiently!



$$f_{NN} = \sigma(b_2 + W_2 \sigma(b_1 + W_1 x))$$

Computational graphs





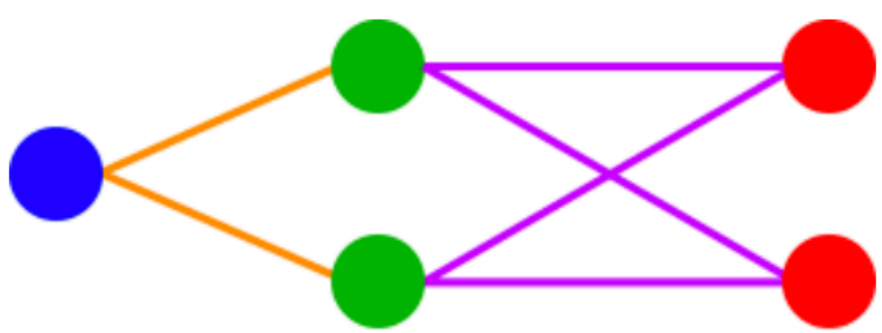
Example neural network → **According computational graph**

- TensorFlow implements all needed **mathematical operations for multi-threaded CPU and multi GPU** environments.
- Computation of neural networks using data flow graphs is a perfect match!

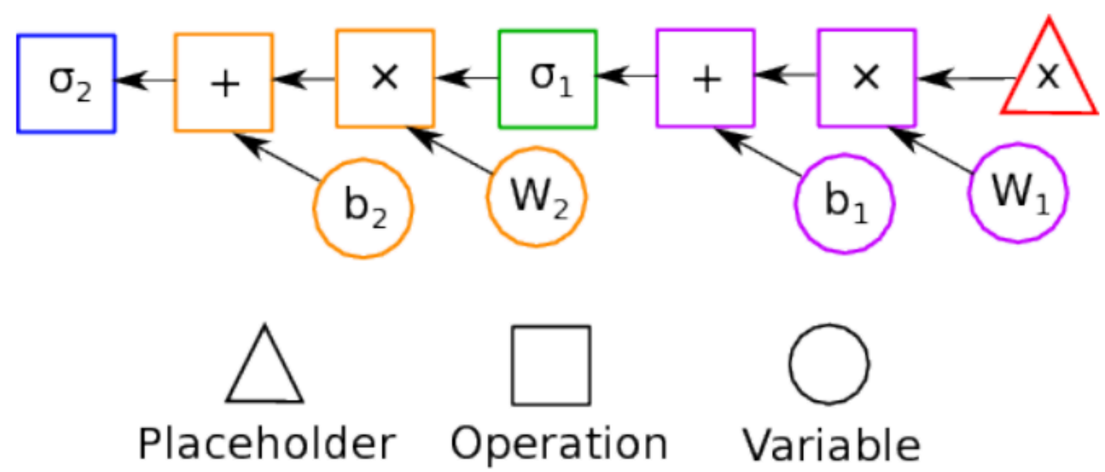
TensorFlow *is an open source software library for numerical computation using data flow graphs.* ***Nodes*** *in the graph* ***represent mathematical operations****, while the* ***graph edges represent the multidimensional data arrays (tensors)*** *communicated between them.*

Basic blocks to build graphs in TensorFlow

- **Basic blocks:**
  - **Placeholders:** Used for injecting data into the graph, e.g., the inputs x of the neural network
  - **Variables:** Free parameters of the graph, e.g., the weight matrices W of the neural network
  - **Operations:** Functions that operate on data in the graph, e.g., the matrix multiplication of W_1 and x



$$f_{NN} = \sigma(b_2 + W_2\sigma(b_1 + W_1 x))$$



Run the graph in a TensorFlow session

- A **graph** in TensorFlow can be run inside a **session**.
- Following example calculates $y = W \cdot x$ using TensorFlow:

Computational graph:

$$y = W \cdot x = \begin{pmatrix} 1 & 2 \end{pmatrix} \cdot \begin{pmatrix} 3 \\ 4 \end{pmatrix} = 11$$

TensorFlow code:

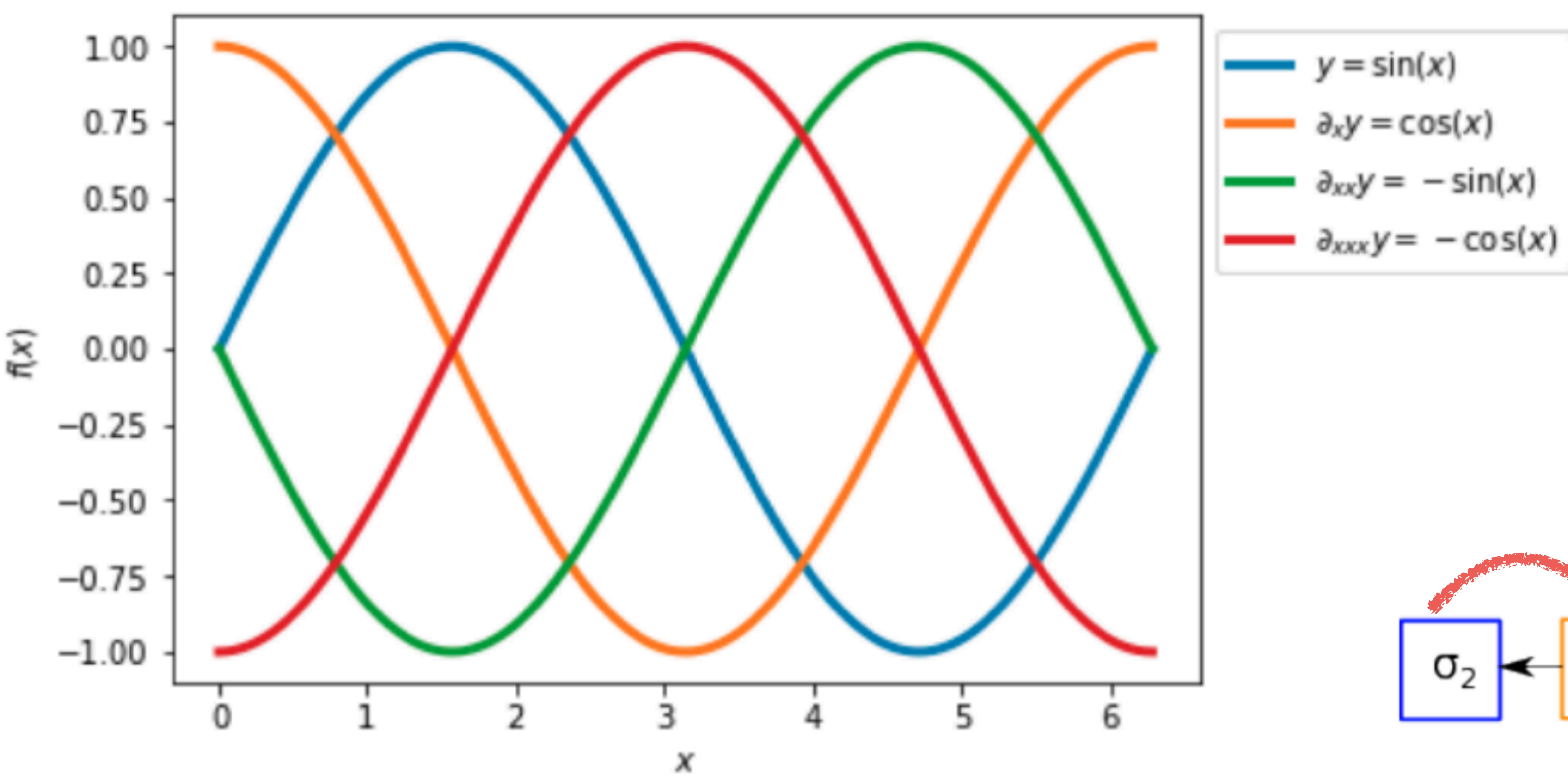
See example: tensorflow/ xor.ipynb

```
import tensorflow as tf
import numpy as np

# Build the graph y = W * x
x = tf.placeholder(tf.float32) # A placeholder
W = tf.get_variable("W", initializer=[[1.0, 2.0]]) # A variable
y = tf.matmul(W, x) # An operation

with tf.Session() as sess: # The session
    sess.run(tf.global_variables_initializer()) # Initialize variables
    result = sess.run(y, feed_dict={x: [[3.0], [4.0]]}) # Run graph
```

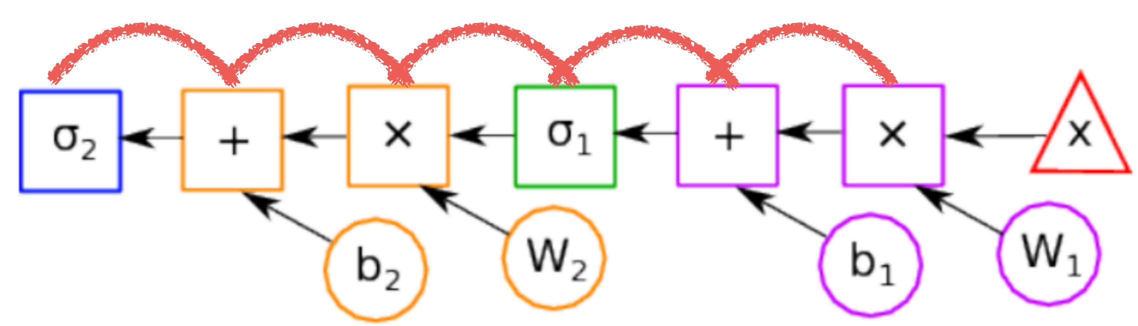
Automatic differentiation

- During training of neural networks make an excessive use of gradients during optimisation
- (Almost) each operation in TensorFlow is shipped with an inbuilt gradient
- Computation of full gradient using the chain-rule of derivatives through the computational graph
- Explicit TensorFlow call: tensorflow.gradients(z, x)

See example: tensorflow/automatic_differentiation.ipynb

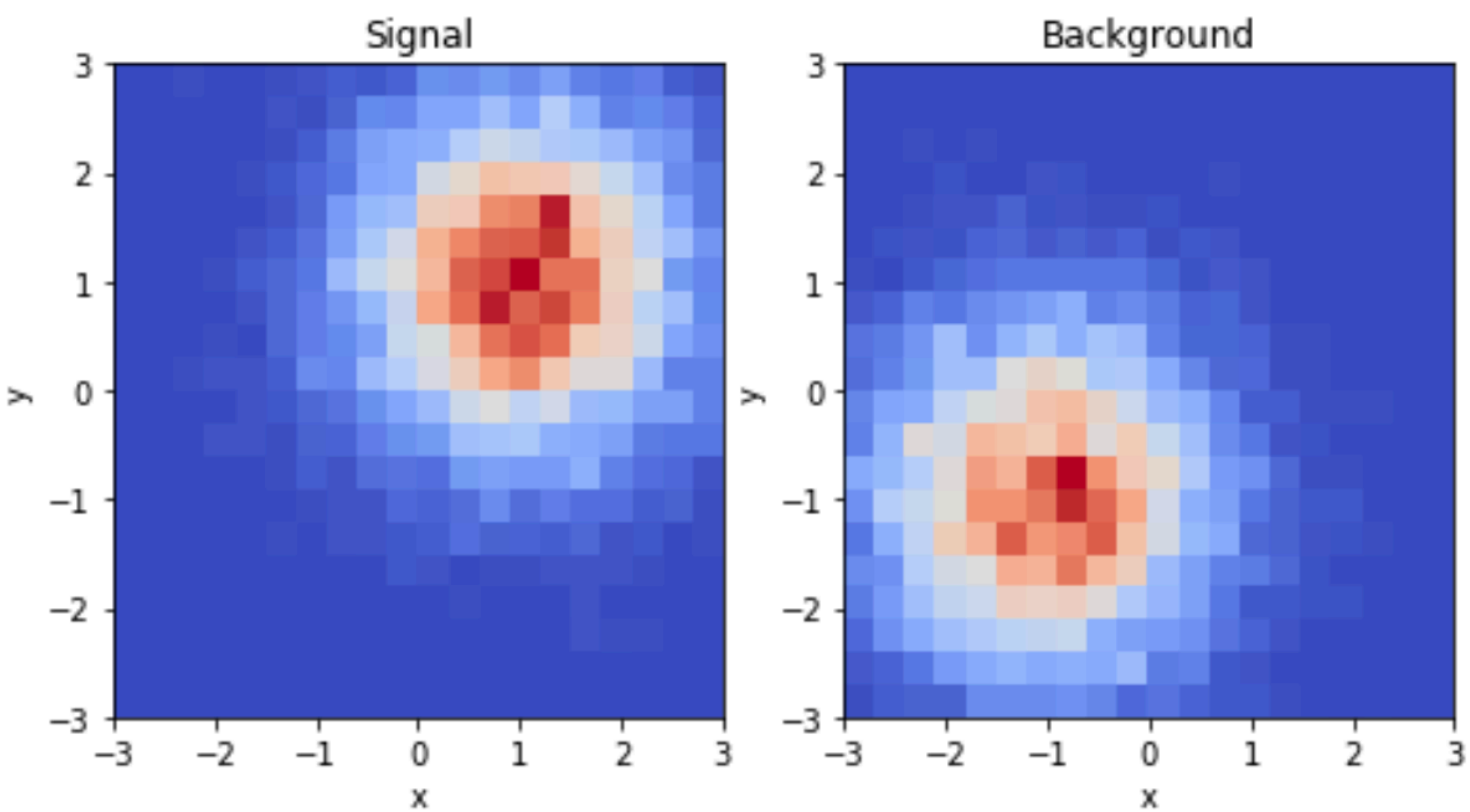


$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}$$



Concrete TensorFlow example: classification of toy Gaussian models

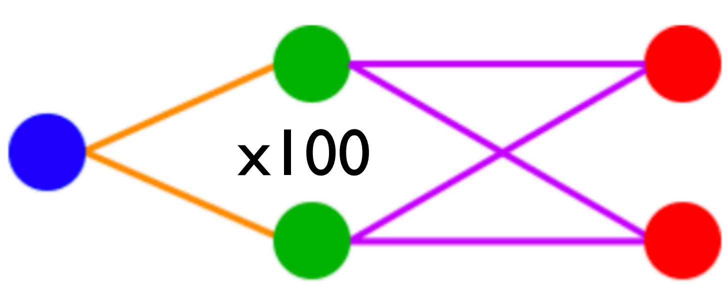
- Carry out a basic classification task separating signal from background
- We will build a single hidden layer neural network with tensor flow and optimise with the Adam gradient descent algorithm



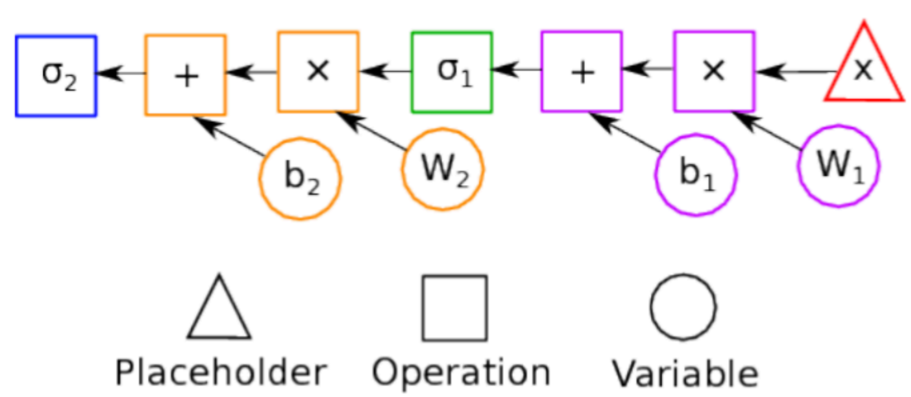
See example: tensorflow/gaussian.ipynb

Define the network architecture

```
In [4]: def model(x):
            with tf.variable_scope("model") as scope:
                w1 = tf.get_variable('w1', shape=(2, 100), dtype=tf.float64,
                        initializer=tf.random_normal_initializer(stddev=0.1))
                b1 = tf.get_variable('b1', shape=(100), dtype=tf.float64,
                        initializer=tf.constant_initializer(0.1))
                w2 = tf.get_variable('w2', shape=(100, 1), dtype=tf.float64,
                        initializer=tf.random_normal_initializer(stddev=0.1))
                b2 = tf.get_variable('b2', shape=(1), dtype=tf.float64,
                        initializer=tf.constant_initializer(0.1))

            l1 = tf.nn.relu(tf.add(b1, tf.matmul(x, w1)))
            logits = tf.add(b2, tf.matmul(l1, w2))
            return logits, tf.sigmoid(logits)

        x = tf.placeholder(tf.float64, shape=[None, 2])
        logits, f = model(x)
```



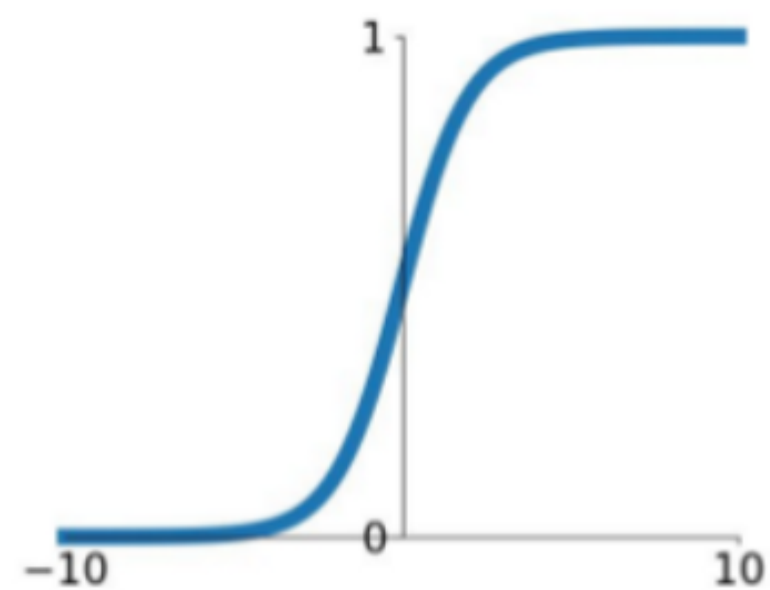
$f_{NN} = \sigma(b_2 + W_2\sigma(b_1 + W_1 x))$



Define the training

- Train using the binary cross entropy calculated on logits
  - Cross entropy usually best choice for classification
    - Equivalent to minimising the negative log likelihood
- Output with a sigmoid activation function
  - Sigmoid trained to 1 for signal and 0 for background
- Use the Adam optimiser: gradient descent with momentum and path correction

$$C = -\frac{1}{n}\sum_x [y \ln a + (1-y)\ln(1-a)],$$



In [5]:
```
labels = tf.placeholder(tf.float64, shape=[None, 1])
loss = tf.reduce_mean(
    tf.nn.sigmoid_cross_entropy_with_logits(labels=labels, logits=logits))
minimize_loss = tf.train.AdamOptimizer().minimize(loss)
```

Compile and run the model

- Everything is done within a TensorFlow session
  - Define this session and call a global variable initialisation
- Pass the predefined loss and loss minimisation procedure to the session, broadcasting the input variables
- Additionally calculate the loss on the test data

In [6]:
```
sess = tf.Session()
sess.run(tf.global_variables_initializer())

loss_train = []
loss_val = []
for i_step in range(100):
    loss_, _ = sess.run([loss, minimize_loss],
                        feed_dict={x: data_train, labels: labels_train})
    loss_train.append(loss_)

    loss_ = sess.run(loss, feed_dict={x: data_val, labels: labels_val})
    loss_val.append(loss_)
```

Extra TensorFlow features

- TensorFlow is designed to perform highly-efficient computations and ships many useful features
  - **Data-loading** often bottleneck if not all data fits in memory (very common for image processing!)
  - TensorFlow provides input pipelines directly inbuilt in the graph
  - Full utilisation of CPU/GPU by loading data form disk in queues in memory concurrently

See example: tensorflow/queues.ipynb

- '**TensorBoard**' can be used for visualisation of graphs
- '**Eager execution**' recently added to emulate PyTorch style
  - https://www.tensorflow.org/guide/eager
- **Keras** provides an excellent high layer wrapper, making development very convenient
- Many more features not mentioned here…

Further reading

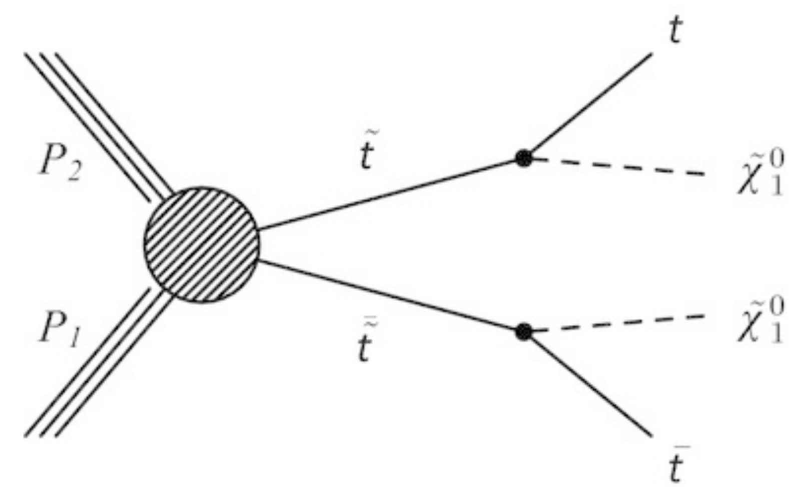
- Stanford course on TensorFlow
  - Very well done and highly entertaining course!
  - Lecturer working in the field (OpenAI, DeepMind, Google, . . .)
  - Small Keras part held by Francois Chollet (author of Keras!)
  - Link: https://web.stanford.edu/class/cs20si/syllabus.html

- Free textbook written by Ian Goodfellow, Yoshua Bengio and Aaron Courville:
  - Leading figures in current machine learning research
  - Covers much of what you could want to know
  - Link: http://www.deeplearningbook.org/

Practice with a physics example

- Now you can try to write your own TensorFlow code in a toy physics scenario
- A background vs signal classification task for a stop SUSY model (with a top anti-top standard model background)

m_{stop}= 600 GeV,
m_{LSP} = 400 GeV



- Try to build a two layer network and train with mini-batch optimisation
- Instructions and skeleton code in tensorflow/physicsExample.ipynb
  - A solution available if you are stuck tensorflow/physicsExample_solution.ipynb
- After this task, have a go at doing a regression task, also in the notebook