

LSML #5

Введение в TensorFlow (SGD для всего)

Chain rule

- We know derivatives for simple functions:

$$\frac{dx^2}{dx} = 2x \qquad \frac{de^x}{dx} = e^x \qquad \frac{d\ln(x)}{dx} = \frac{1}{x}$$

- Let's take a composite function:

$$z_1 = z_1(\textcolor{red}{x}_1, x_2)$$

$$z_2 = z_2(\textcolor{green}{x}_1, x_2) \qquad \text{where } z_1, z_2, p \text{ are differentiable}$$

$$p = p(\textcolor{violet}{z}_1, \textcolor{green}{z}_2)$$

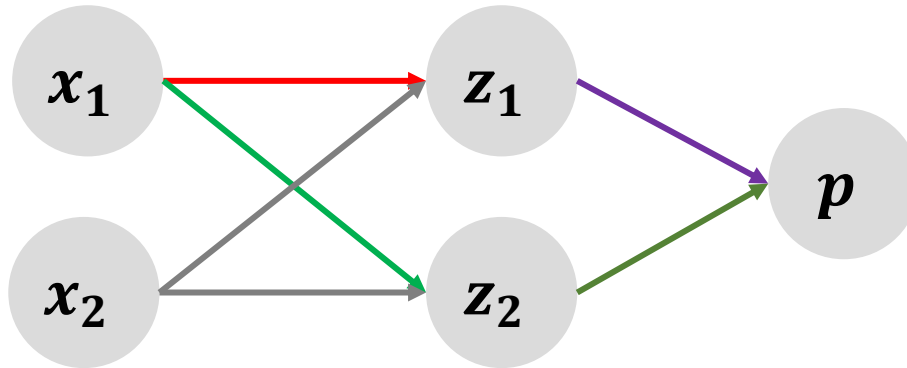
$$\text{Chain rule: } \frac{\partial p}{\partial x_1} = \frac{\partial p}{\partial \textcolor{violet}{z}_1} \frac{\partial \textcolor{red}{z}_1}{\partial \textcolor{red}{x}_1} + \frac{\partial p}{\partial \textcolor{green}{z}_2} \frac{\partial \textcolor{green}{z}_2}{\partial \textcolor{green}{x}_1}$$

Example for $h(x) = f(x)g(x)$:

$$\frac{\partial h}{\partial x} = \frac{\partial h}{\partial f} \frac{\partial f}{\partial x} + \frac{\partial h}{\partial g} \frac{\partial g}{\partial x} = \textcolor{blue}{g} \frac{\partial f}{\partial x} + \textcolor{pink}{f} \frac{\partial g}{\partial x}$$

Derivatives computation graph

- Let's take a simple MLP:

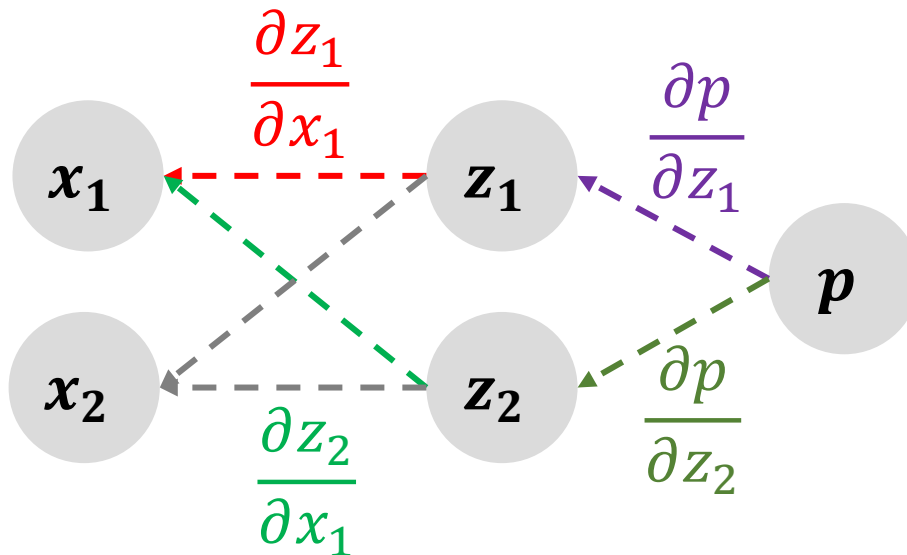


$$z_1 = z_1(x_1, x_2)$$

$$z_2 = z_2(x_1, x_2)$$

$$p = p(z_1, z_2)$$

- And construct a new graph of derivatives:



$$\frac{\partial p}{\partial x_1} = \frac{\partial p}{\partial z_1} \frac{\partial z_1}{\partial x_1} + \frac{\partial p}{\partial z_2} \frac{\partial z_2}{\partial x_1}$$

Each edge is assigned
to derivative of origin
w.r.t. destination

Let's look at MLP

3: $\frac{\partial p}{\partial h_1}$ $\frac{\partial p}{\partial h_2}$

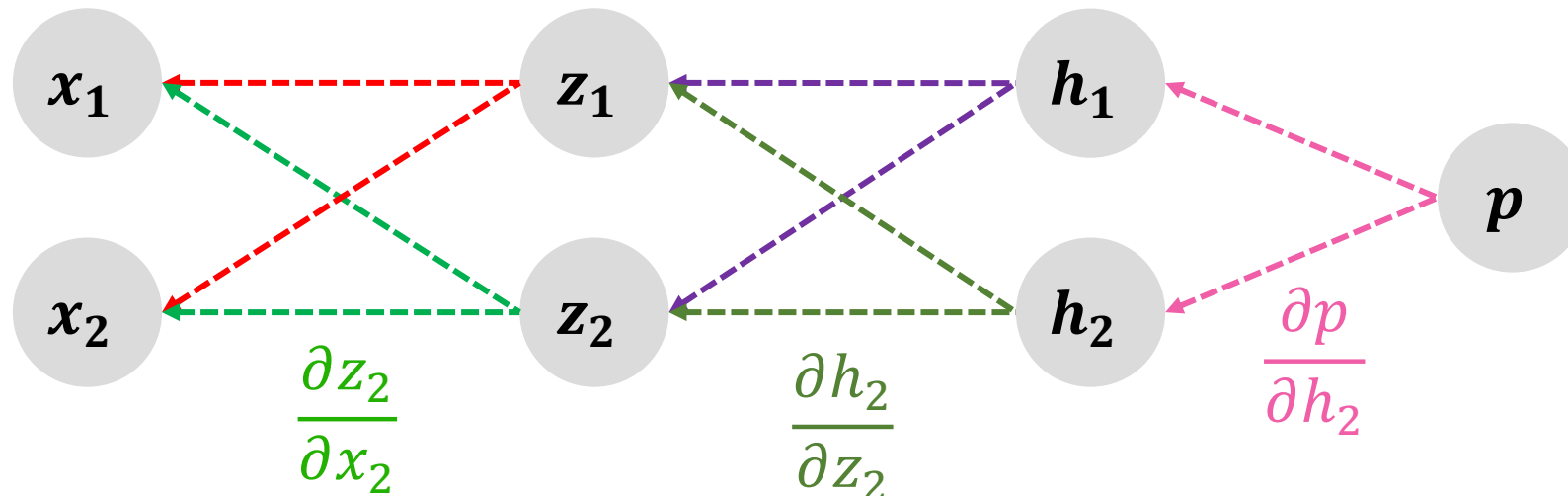
All the derivatives we need for SGD

2: $\frac{\partial p}{\partial z_1} = \frac{\partial p}{\partial h_1} \frac{\partial h_1}{\partial z_1} + \frac{\partial p}{\partial h_2} \frac{\partial h_2}{\partial z_1}$

$\frac{\partial p}{\partial z_2} = \frac{\partial p}{\partial h_1} \frac{\partial h_1}{\partial z_2} + \frac{\partial p}{\partial h_2} \frac{\partial h_2}{\partial z_2}$

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$\frac{\partial p}{\partial x_2} = \frac{\partial p}{\partial h_1} \frac{\partial h_1}{\partial z_1} \frac{\partial z_1}{\partial x_2} + \frac{\partial p}{\partial h_2} \frac{\partial h_2}{\partial z_1} \frac{\partial z_1}{\partial x_2} + \frac{\partial p}{\partial h_1} \frac{\partial h_1}{\partial z_2} \frac{\partial z_2}{\partial x_2} + \frac{\partial p}{\partial h_2} \frac{\partial h_2}{\partial z_2} \frac{\partial z_2}{\partial x_2}$



We can reuse previous computations

3: $\frac{\partial p}{\partial h_1}$ $\frac{\partial p}{\partial h_2}$

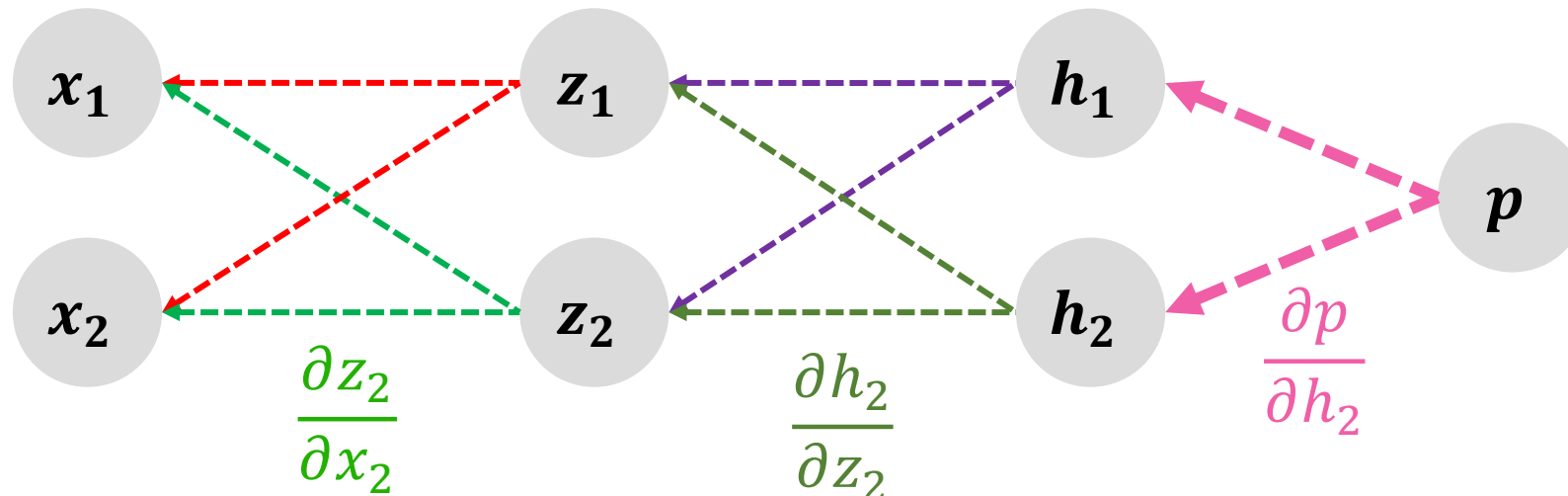
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$\frac{\partial p}{\partial x_2} = \frac{\partial p}{\partial h_1} \frac{\partial h_1}{\partial z_1} \frac{\partial z_1}{\partial x_2} + \frac{\partial p}{\partial h_2} \frac{\partial h_2}{\partial z_1} \frac{\partial z_1}{\partial x_2} + \frac{\partial p}{\partial h_1} \frac{\partial h_1}{\partial z_2} \frac{\partial z_2}{\partial x_2} + \frac{\partial p}{\partial h_2} \frac{\partial h_2}{\partial z_2} \frac{\partial z_2}{\partial x_2}$



We can reuse previous computations

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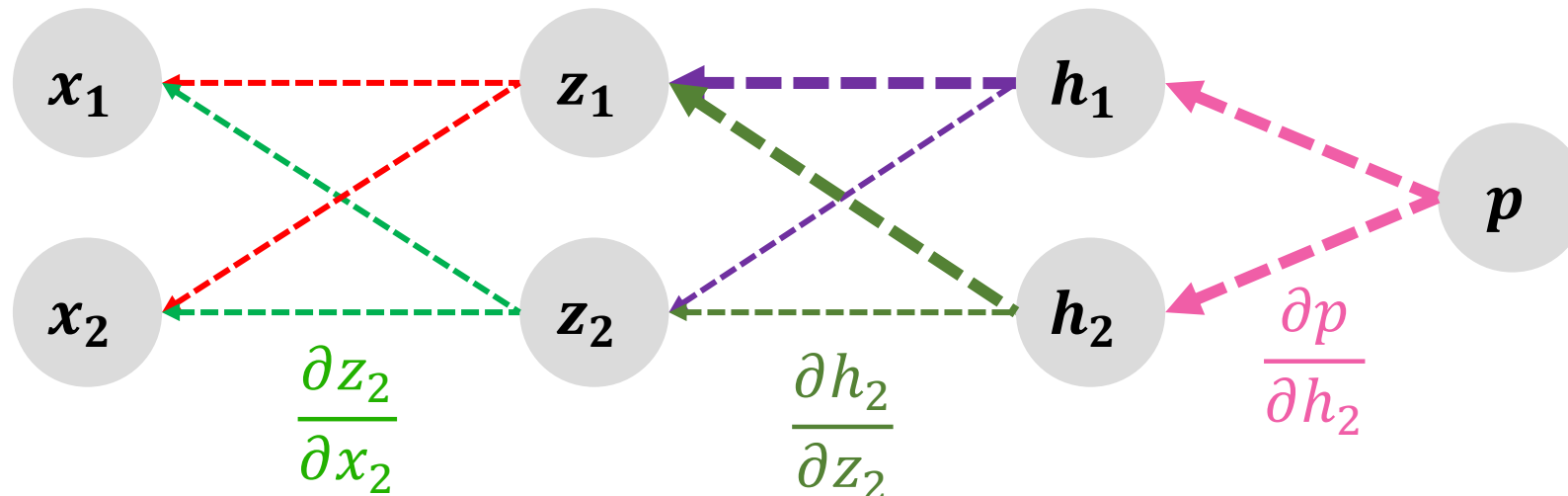
All the derivatives we need for SGD

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We can reuse previous computations

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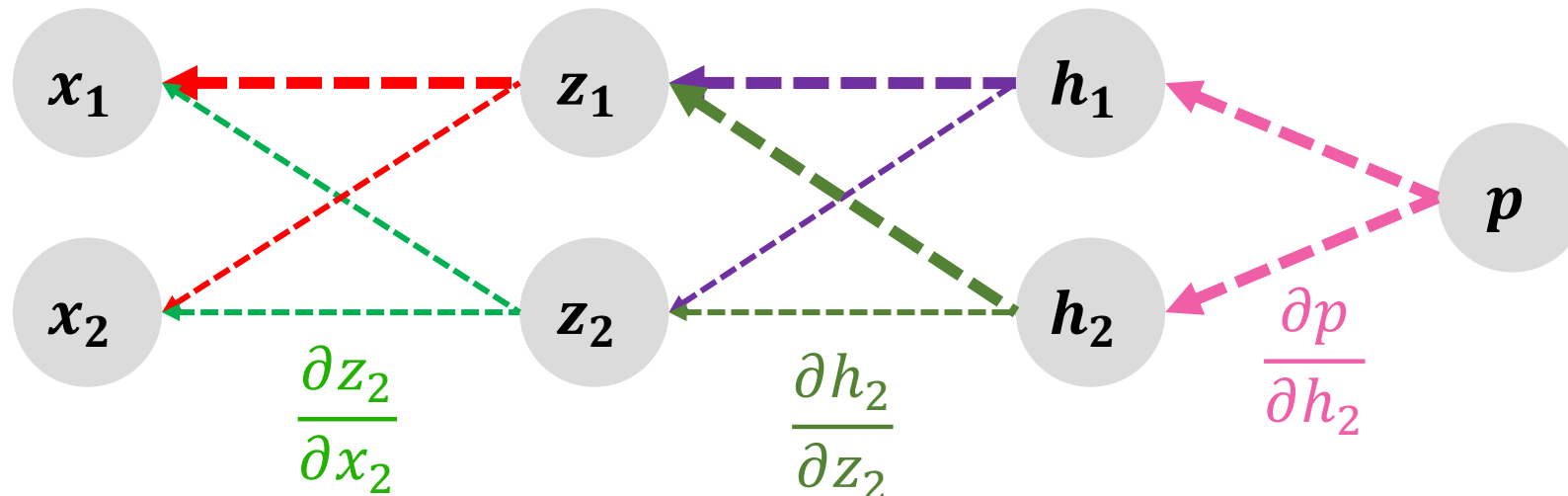
All the derivatives we need for SGD

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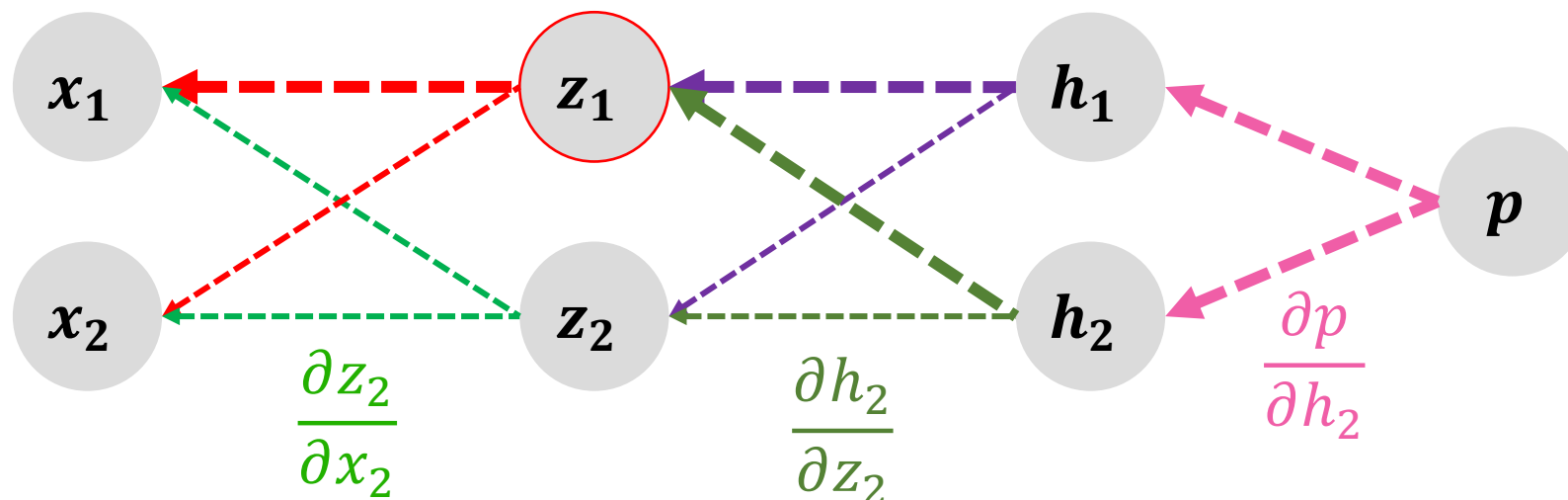
We can reuse previous computations

3: $\frac{\partial p}{\partial h_1}$ $\frac{\partial p}{\partial h_2}$ All the derivatives we need for SGD

2: $\frac{\partial p}{\partial z_1} = \frac{\partial p}{\partial h_1} \frac{\partial h_1}{\partial z_1} + \frac{\partial p}{\partial h_2} \frac{\partial h_2}{\partial z_1}$ $\frac{\partial p}{\partial z_2} = \frac{\partial p}{\partial h_1} \frac{\partial h_1}{\partial z_2} + \frac{\partial p}{\partial h_2} \frac{\partial h_2}{\partial z_2}$

1: $\frac{\partial p}{\partial x_1} = \left(\frac{\partial p}{\partial h_1} \frac{\partial h_1}{\partial z_1} + \frac{\partial p}{\partial h_2} \frac{\partial h_2}{\partial z_1} \right) \frac{\partial z_1}{\partial x_1} + \frac{\partial p}{\partial h_1} \frac{\partial h_1}{\partial z_2} \frac{\partial z_2}{\partial x_1} + \frac{\partial p}{\partial h_2} \frac{\partial h_2}{\partial z_2} \frac{\partial z_2}{\partial x_1}$

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We can reuse previous computations

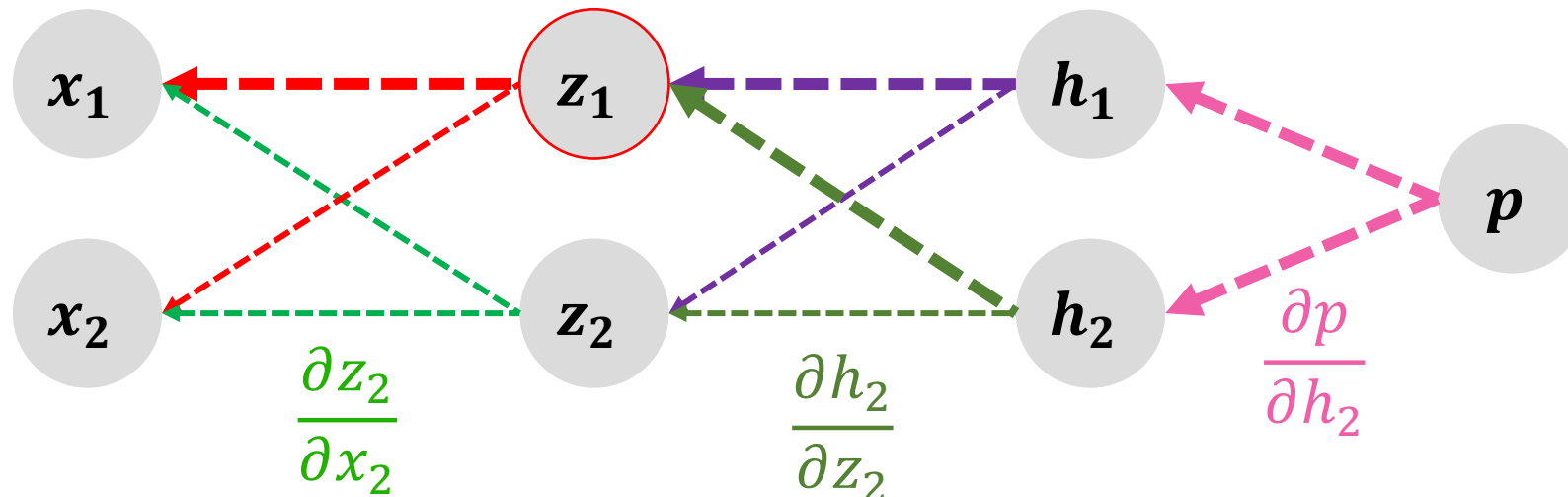
3: $\frac{\partial p}{\partial h_1}$ $\frac{\partial p}{\partial h_2}$

All the derivatives we need for SGD

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1: $\frac{\partial p}{\partial x_1} = \left(\frac{\partial p}{\partial z_1} \right) \frac{\partial z_1}{\partial x_1} + \frac{\partial p}{\partial h_1} \frac{\partial h_1}{\partial z_2} \frac{\partial z_2}{\partial x_1} + \frac{\partial p}{\partial h_2} \frac{\partial h_2}{\partial z_2} \frac{\partial z_2}{\partial x_1}$

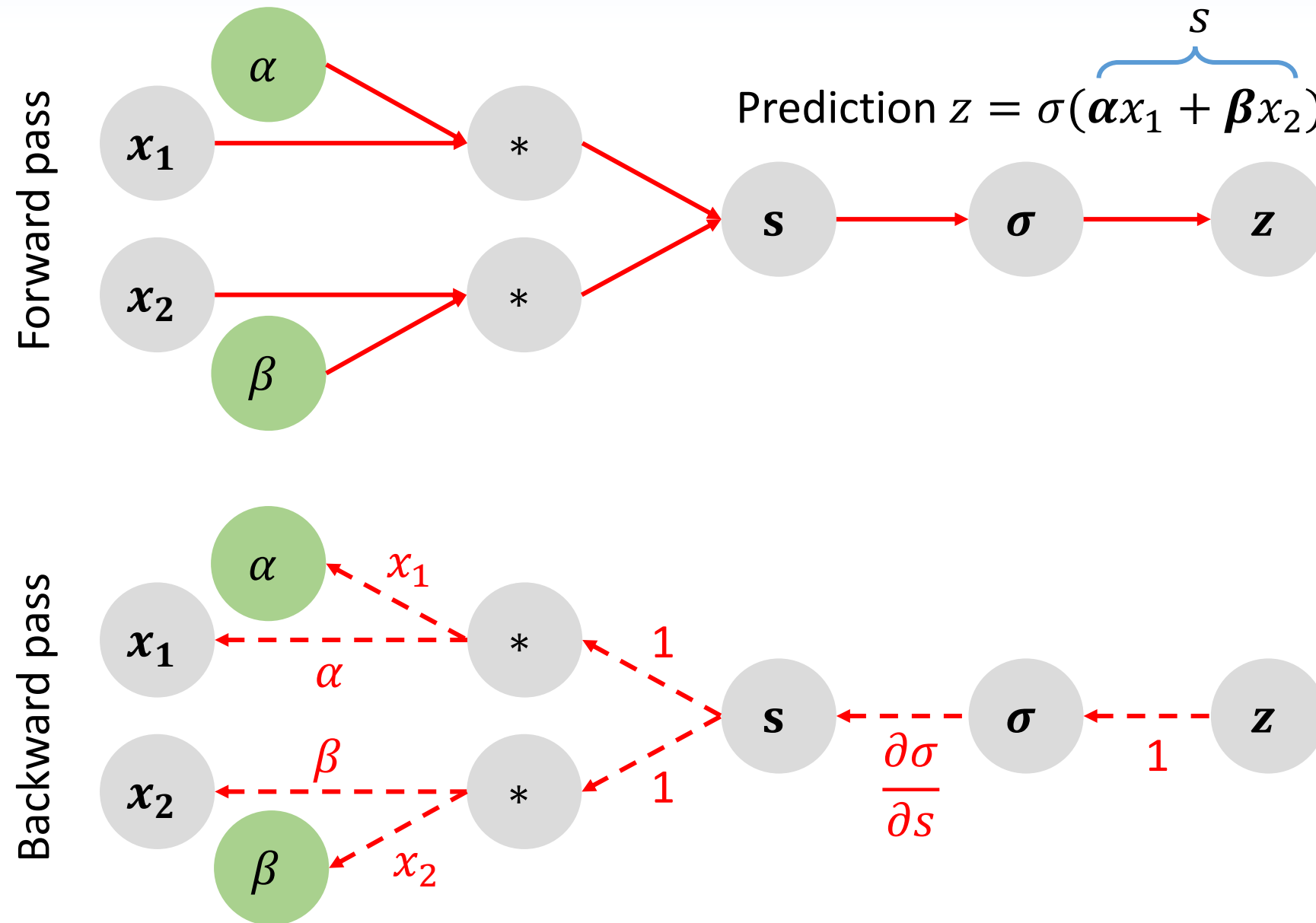
$\frac{\partial p}{\partial x_2} = \frac{\partial p}{\partial h_1} \frac{\partial h_1}{\partial z_1} \frac{\partial z_1}{\partial x_2} + \frac{\partial p}{\partial h_2} \frac{\partial h_2}{\partial z_1} \frac{\partial z_1}{\partial x_2} + \frac{\partial p}{\partial h_1} \frac{\partial h_1}{\partial z_2} \frac{\partial z_2}{\partial x_2} + \frac{\partial p}{\partial h_2} \frac{\partial h_2}{\partial z_2} \frac{\partial z_2}{\partial x_2}$



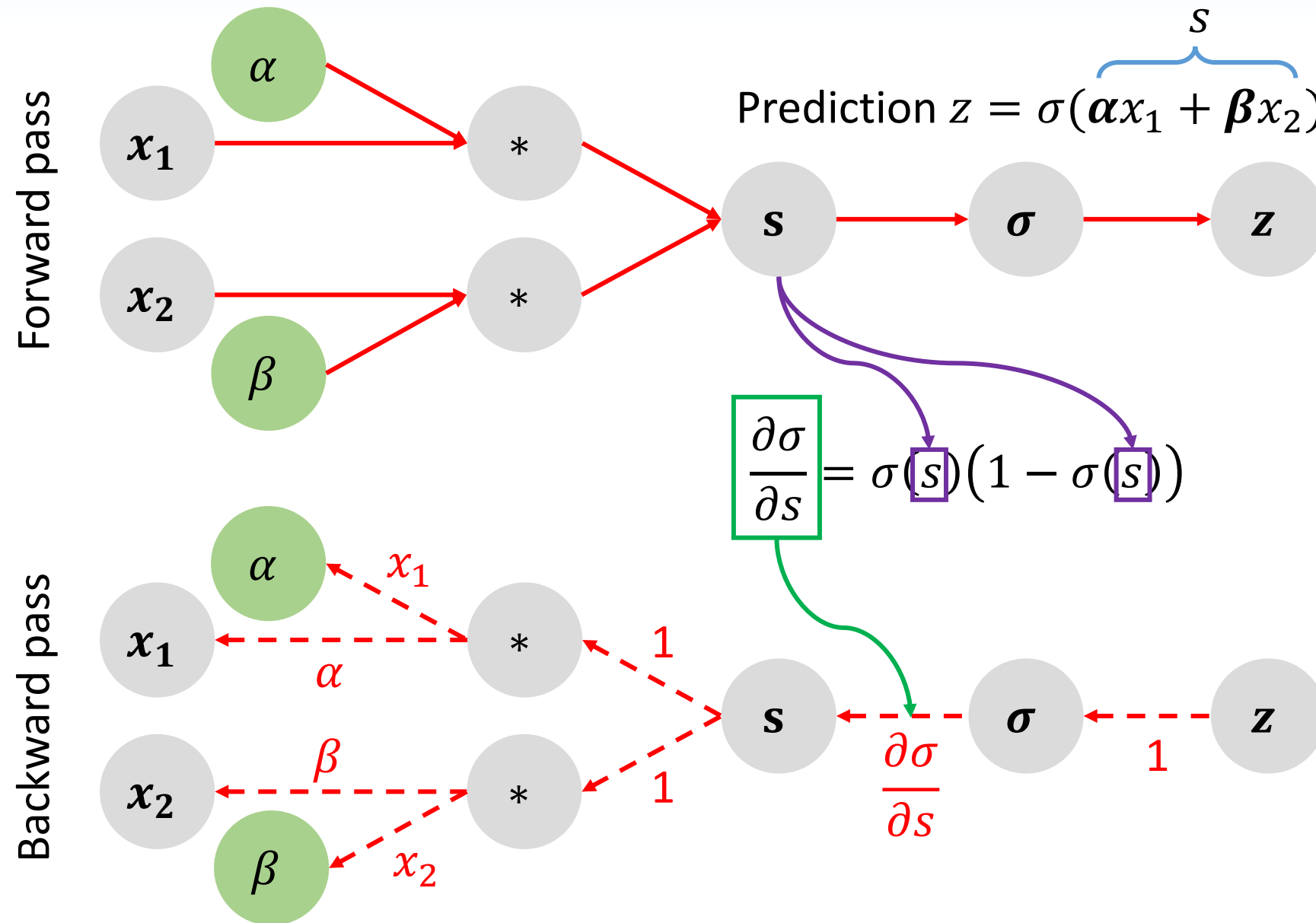
This is called reverse-mode differentiation

- In application to neural networks it has one more name: **back-propagation**.
- It works **fast**, because we reuse computations from previous steps.
- In fact, for each edge we compute its value only once. And multiply by its value exactly once.

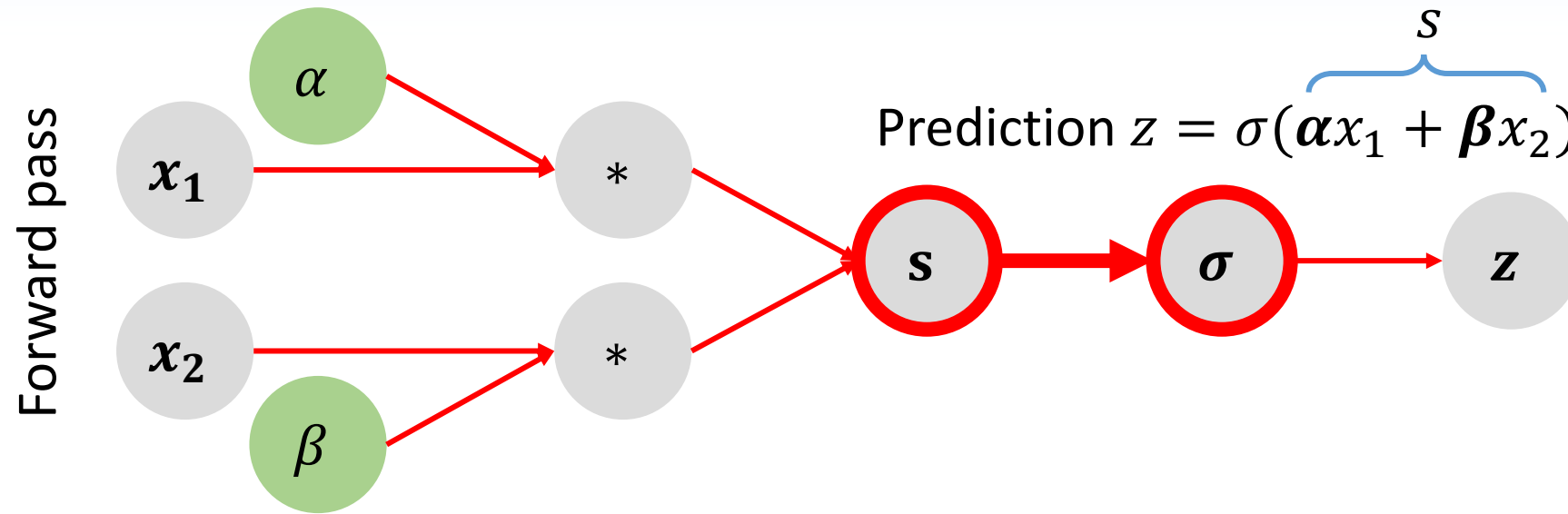
Back-propagation (Back-prop)



Back-propagation (Back-prop)

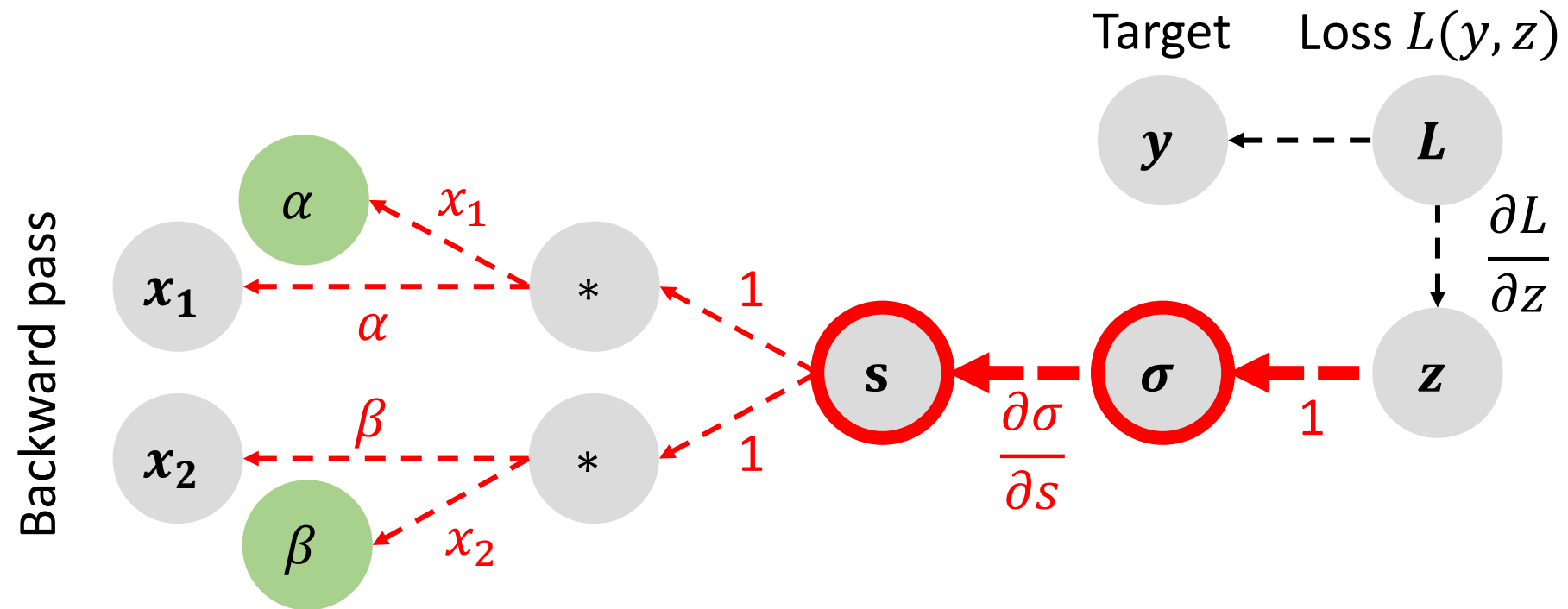


Forward pass interface

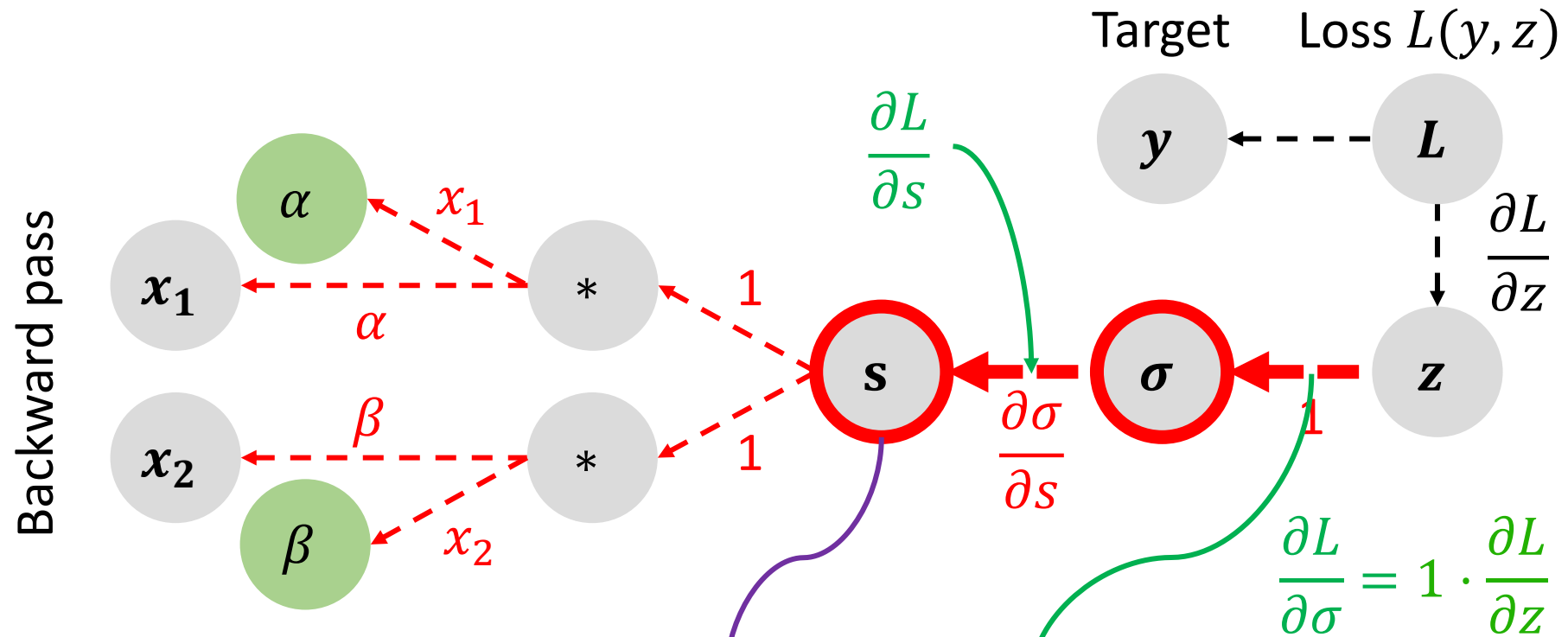


```
def forward_pass(inputs):  
    return 1. / (1 + np.exp(-inputs))
```

Backward pass interface



Backward pass interface



```
def backward_pass(inputs, incoming_gradient):  
    sigmoid = 1. / (1 + np.exp(-inputs))  
    return sigmoid * (1 - sigmoid) * incoming_gradient
```

$$\frac{\partial L}{\partial s}$$

=

$$\frac{\partial \sigma}{\partial s}$$

.

$$\frac{\partial L}{\partial \sigma}$$

TensorFlow DL framework

- We will use it in Jupyter Notebook with Python kernel

```
import numpy as np  
import tensorflow as tf
```

- We will overview Python API for TensorFlow 1.2+
- APIs in other languages exist: Java, C++, Go
 - Python API is at present the most complete and the easiest to use
 - https://www.tensorflow.org/api_docs/



What is TensorFlow?

1. A tool to describe computational graphs
 - The foundation of computation in TensorFlow is the **Graph** object. This holds a network of nodes, each representing one **operation**, connected to each other as inputs and outputs.
2. A runtime for execution of these graphs
 - On CPU, GPU, TPU, ...
 - On one node or in distributed mode



Why this name

- **Input** to any operation will be a collection of **tensors** (multi-dimensional arrays)
- **Output** will be a collection of tensors as well.
- We will have a graph of operations, which transforms tensors into another tensors, so it's a kind of a flow of tensors 😊

How input looks like

- **Placeholder**

- This is placeholder for a tensor, which will be fed during graph execution (e.g. input features)
- `x = tf.placeholder(tf.float32, (None, 10))`

- **Variable**

- This is a tensor with some value that is updated during execution (e.g. weights matrix in MLP)
- `w = tf.get_variable("w", shape=(10, 20), dtype=tf.float32)`
- `w = tf.Variable(tf.random_uniform((10, 20)), name="w")`

- **Constant**

- This is a tensor with constant value, that cannot be changed
- `c = tf.constant(np.ones((4, 4)))`

Operation example

- Matrix product:

```
x = tf.placeholder(tf.float32, (None, 10))
w = tf.Variable(tf.random_uniform((10, 20)), name="w")
z = x @ w
# z = tf.matmul(x, w)
print(z)
```

- Output:

Tensor("matmul:0", shape=(?, 20), dtype=float32)

- We don't do any computations here, we just **define** the graph!

Computational graph

- TensorFlow creates a **default graph** after importing
 - All the operations will go there by default
 - You can get it with `tf.get_default_graph()`, which returns an instance of `tf.Graph`.
- You can **create your own** graph variable and define operations there:

```
g = tf.Graph()  
with g.as_default():  
    pass
```

- You can **clear** the default graph like this:

```
tf.reset_default_graph()
```

Jupyter Notebook cells

- If you run this cell **3 times**:

```
x = tf.placeholder(tf.float32, (None, 10))
```

- This is what you get in your **default graph**:

- Using `tf.get_default_graph().get_operations()`

```
[<tf.Operation 'Placeholder' type=Placeholder>,  
<tf.Operation 'Placeholder_1' type=Placeholder>,  
<tf.Operation 'Placeholder_2' type=Placeholder>]
```

- **Your graph is cluttered!**

- Clear your graph with `tf.reset_default_graph()` before changing

Operations and tensors

- Every **node** in our graph is an **operation**:

```
x = tf.placeholder(tf.float32, (None, 10), name="x")
```

- Listing nodes with `tf.get_default_graph().get_operations()`:

```
[<tf.Operation 'x' type=Placeholder>]
```

- How to get **output tensors** of operation:

- `tf.get_default_graph().get_operations()[0].outputs`

- Output: `[<tf.Tensor 'x:0' shape=(?, 10) dtype=float32>]`

Running a graph

- A **tf.Session** object encapsulates the environment in which `tf.Operation` objects are executed, and `tf.Tensor` objects are evaluated.

- Create a session:

```
s = tf.InteractiveSession()
```

- Defining a graph:

```
a = tf.constant(5.0)
```

```
b = tf.constant(6.0)
```

```
c = a * b
```

- Running a graph:

```
print(c) # here just looking at the type
```

```
print(s.run(c)) # that's how you run the graph
```

- Output:

```
Tensor("mul:0", shape=(), dtype=float32)
```

```
30.0
```


Running a graph

- Operations are written in C++ and executed on CPU or GPU.
- `tf.Session` owns necessary resources to execute your graph, such as `tf.Variable`, that occupy RAM.
- It is important to release these resources when they are no longer required with `tf.Session.close()`

Initialization of variables

- A variable has an initial value:
 - Tensor: `tf.Variable(tf.random_uniform((10, 20)), name="w")`
 - Initializer: `tf.get_variable("w", shape=(10, 20), dtype=tf.float32)`
- You need to run some code to **compute that initial value** in graph execution environment
- This is done with a call in your session `s`:

```
s.run(tf.global_variables_initializer())
```
- Without it you will get “Attempting to use uninitialized value” errors

Example

- Definition:

```
tf.reset_default_graph()
a = tf.constant(np.ones((2, 2), dtype=np.float32))
b = tf.Variable(tf.ones((2, 2)))
c = a @ b
```

- Running attempt:

```
s = tf.InteractiveSession()
s.run(c)
```

Output: “Attempting to use uninitialized value” error

- Running properly:

```
s.run(tf.global_variables_initializer())
s.run(c)
```

Output: array([[2., 2.], [2., 2.]], dtype=float32)

Feeding placeholder values

- Definition:

```
tf.reset_default_graph()
a = tf.placeholder(np.float32, (2, 2))
b = tf.Variable(tf.ones((2, 2)))
c = a @ b
```

- Running attempt:

```
s = tf.InteractiveSession()
s.run(tf.global_variables_initializer())
s.run(c)
```

Output: **“You must feed a value for placeholder tensor”** error

- Running properly:

```
s.run(tf.global_variables_initializer())
s.run(c, feed_dict={a: np.ones((2, 2))})
```

Output: array([[2., 2.], [2., 2.]], dtype=float32)

Summary

- TensorFlow: defining and running computational graphs
- Nodes of a graph are operations, that convert a collection of tensors into another collection of tensors
- In Python API you **define** the graph, you **don't execute** it along the way
 - In 1.5+ the latter mode is supported: eager execution
- You create a **session** to execute your graph (fast C++ code on CPU or GPU)
- Session **owns** all the resources (tensors eat RAM)

Optimizers in TensorFlow

- Let's define **f** as a square of variable **x**:

```
import numpy as np
import tensorflow as tf

tf.reset_default_graph()
x = tf.get_variable("x", shape=(), dtype=tf.float32)
f = x ** 2
```

- Let's say we want to *minimize* the value of **f** w.r.t **x**:

```
optimizer = tf.train.GradientDescentOptimizer(0.1)
step = optimizer.minimize(f, var_list=[x])
```

Trainable variables

- You don't have to specify all the optimized variables:

```
step = optimizer.minimize(f, var_list=[x])  
step = optimizer.minimize(f)
```

- Because all variables are **trainable** by default:

```
x = tf.get_variable("x", shape=(), dtype=tf.float32)  
x = tf.get_variable("x", shape=(), dtype=tf.float32, trainable=True)
```

- You can get all of them:

```
tf.trainable_variables()
```

- Output:

```
[<tf.Variable 'x:0' shape=() dtype=float32_ref>]
```

Making gradient descent steps

- Now we need to create a **session** and **initialize** variables:

```
s = tf.InteractiveSession()  
s.run(tf.global_variables_initializer())
```

- We are ready to make 10 **gradient descent** steps:

```
for i in range(10):  
    _, curr_x, curr_f = s.run([step, x, f])  
    print(curr_x, curr_f)
```

- Output:

```
0.448929 0.314901  
0.359143 0.201537  
...  
0.0753177 0.00886368  
0.0602542 0.00567276
```

← *GD step is already
applied to x*

Logging with tf.Print

- We can **evaluate** tensors and print them like this:

```
for i in range(10):  
    _, curr_x, curr_f = s.run([step, x, f])  
    print(curr_x, curr_f)
```

- Or we can pass our tensor of interest through **tf.Print**:

```
...  
f = x ** 2  
f = tf.Print(f, [x, f], "x, f:")  
...  
for i in range(10):  
    s.run([step, f])
```

```
x, f:[1.5879565][2.521606]  
x, f:[1.2703652][1.6138278]  
...  
x, f:[0.26641488][0.070976891]  
x, f:[0.2131319][0.04542521]
```

*This is Jupyter Server stdout.
Not visible in the Notebook!*

Logging with TensorBoard


- We can add so-called **summaries**:

```
tf.summary.scalar('curr_x', x)
tf.summary.scalar('curr_f', f)
summaries = tf.summary.merge_all()
```

- This is how we log these summaries:

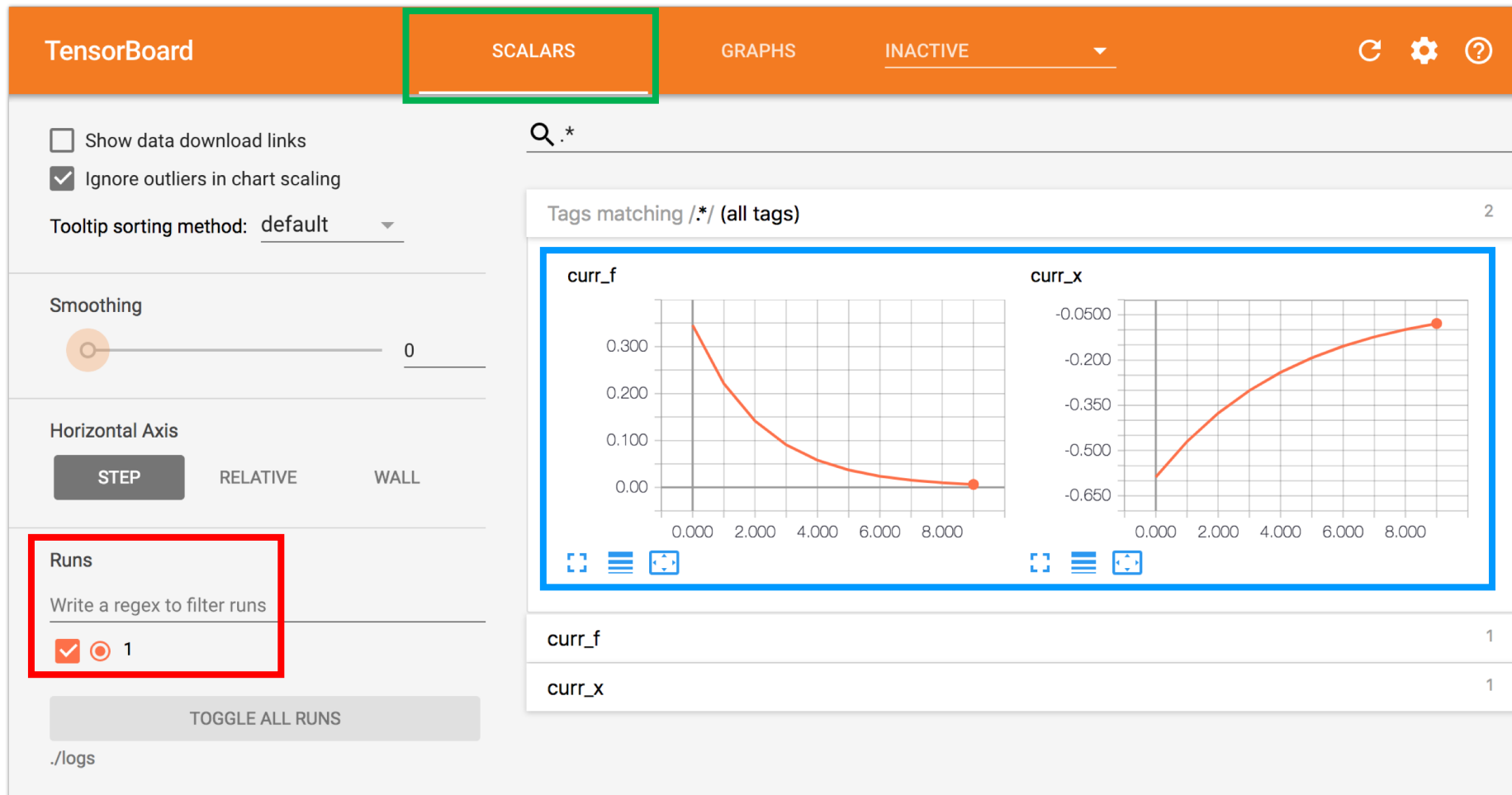
```
s = tf.InteractiveSession()
summary_writer = tf.summary.FileWriter("logs/1", s.graph)
s.run(tf.global_variables_initializer())
for i in range(10):
    _, curr_summaries = s.run([step, summaries])
    summary_writer.add_summary(curr_summaries, i)
    summary_writer.flush()
```

Run number



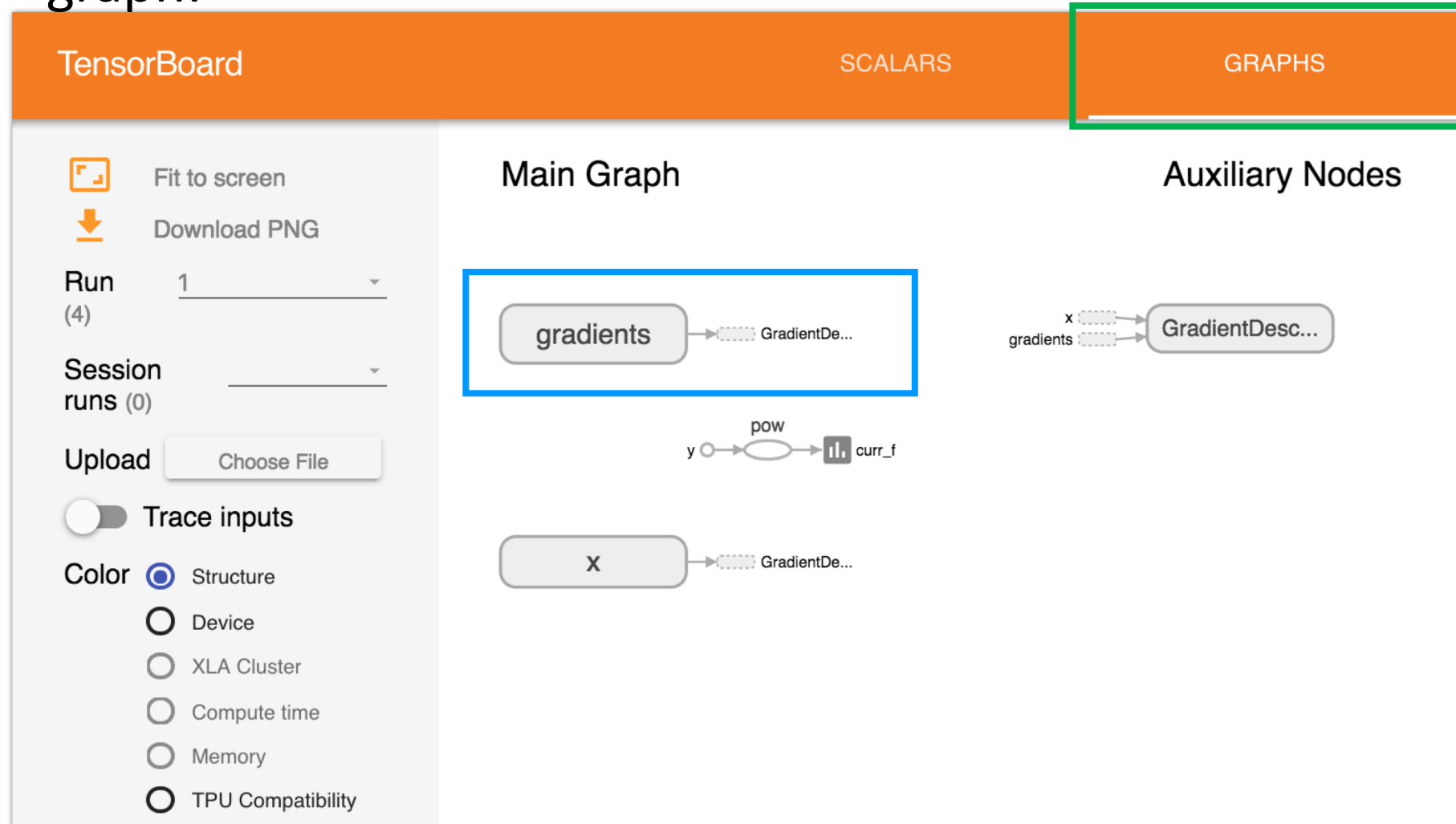
Launching TensorBoard

- Now you can launch TensorBoard via bash:
`tensorboard --logdir=./logs`
- And open **`http://127.0.0.1:6006`** in your browser.



Visualizing graph in TensorBoard

- You can see that **gradients computation** is a part of our graph:



Solving a linear regression

- Let's generate a model dataset:

$N = 1000$

$D = 3$

$x = \text{np.random.random}((N, D))$

$w = \text{np.random.random}(D, 1)$

$y = x @ w + \text{np.random.randn}(N, 1) * 0.20$

Solving a linear regression

- We will need **placeholders** for input data:

```
tf.reset_default_graph()
features = tf.placeholder(tf.float32, shape=(None, D))
target = tf.placeholder(tf.float32, shape=(None, 1))
```

- This is how we make **predictions**:

```
weights = tf.get_variable("weights", shape=(D, 1), dtype=tf.float32)
predictions = features @ weights
```

- And define our **loss**:

```
loss = tf.reduce_mean((target - predictions) ** 2)
```

- And **optimizer**:


```
optimizer = tf.train.GradientDescentOptimizer(0.1)
step = optimizer.minimize(loss)
```

Solving a linear regression

- Gradient descent:

```
s = tf.InteractiveSession()
s.run(tf.global_variables_initializer())
for i in range(300):
    _, curr_loss, curr_weights = s.run(
        [step, loss, weights], feed_dict={features: x, target: y})
    if i % 50 == 0:
        print(curr_loss)
```

Filling placeholders



- Ground truth weights:

[0.11649134,0.82753164,0.46924019]

- Found weights:

[0.13715988,0.79555332,0.47024861]

Model checkpoints

- We can save variables' state with **tf.train.Saver**:

```
s = tf.InteractiveSession()
saver = tf.train.Saver(tf.trainable_variables())
s.run(tf.global_variables_initializer())
for i in range(300):
    _, curr_loss, curr_weights = s.run(
        [step, loss, weights], feed_dict={features: x, target: y})
    if i % 50 == 0:
        saver.save(s, "logs/2/model.ckpt", global_step=i)
    print(curr_loss)
```


Model checkpoints

- We can **list** last checkpoints:

```
saver.last_checkpoints  
  
['logs/2/model.ckpt-50', 'logs/2/model.ckpt-100',  
'logs/2/model.ckpt-150', 'logs/2/model.ckpt-200',  
'logs/2/model.ckpt-250']
```

- We can **restore** a previous checkpoint like this:

```
saver.restore(s, "logs/2/model.ckpt-50")
```

- Only variables' values are restored, which means that you need to define a graph in *the same* way **before restoring** a checkpoint.

Summary

- TensorFlow has **built-in optimizers** that do back-propagation automatically.
- TensorBoard provides **tools for visualizing** your training progress.
- TensorFlow allows you to **checkpoint** your graph to restore its state later (*you need to define it in exactly the same way though*)

Целая программа на TF

```
import tensorflow as tf
import numpy as np
```

Импортировали TF

```
trX = np.linspace(-1, 1, 101)
trY = 2 * trX + np.random.randn(*trX.shape) * 0.33
```

Сгенерировали тестовые данные

```
x = tf.placeholder("float")
y = tf.placeholder("float")
w = tf.Variable(0.0, name="weights")

y_pred = tf.multiply(x, w)
loss = tf.square(y - y_pred)
train_step = tf.train.GradientDescentOptimizer(0.01).minimize(loss)
```

Создали переменные для графа

*Наша модель – $x * w$*

Функция потерь

Шаг по градиенту loss

```
with tf.Session() as sess:
    tf.global_variables_initializer().run()
    for i in range(10):
        for (_x, _y) in zip(trX, trY):
            sess.run(train_step, feed_dict={x: _x, y: _y})
    print(sess.run(w))
```

Создали сессию

Инициализировали переменные

Делаем шаг по градиенту loss

Получаем результирующий w

2.04825

То же самое на Keras (библиотека поверх TF)

```
import tensorflow as tf
import tensorflow.contrib.keras as keras
import numpy as np
```

```
trX = np.linspace(-1, 1, 101)
trY = 2 * trX + np.random.randn(*trX.shape) * 0.33
```

```
model = keras.models.Sequential()
model.add(keras.layers.Dense(1, input_shape=(1,)))
model.compile(optimizer='sgd', loss='mse', metrics=['mse'])
```

```
model.fit(trX, trY, batch_size=1, epochs=10, verbose=0)
model.get_weights()
```

```
[array([[ 2.11763072]]), dtype=float32), array([-0.02399813], dtype=float32)]
```

Ссылки

- TensorFlow tutorials <https://www.tensorflow.org/tutorials>