Big Data Analytics

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C. Distributed Computing Environments / 3. Computational Graphs (TensorFlow)

Syllabus

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2. Variables
3. Example: Linear Regression
4. Automatic Gradients
5. Large Data I: Feeding
6. Large Data II: Reader Nodes
7. Debugging

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1. The Computational Graph

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TensorFlow

- Computational framework
- multi-device, distributed
- Core in C/C++, standard interface in Python
  - several further language bindings, e.g., R, Java
- open source
  - developed by Google
  - initially released Nov. 2015
  - 2nd generation framework
    - 1st generation framework was called DistBelief
- alternative: pytorch
  - developed by facebook, since 2016, open source

Tensors

- tensor = multidimensional array
  - rank = number of dimensions
  - shape = vector of sizes,
    one size for each dimension.

rank	common name	shape
0	scalar	()
1	vector	(size)
2	matrix	(numrows, numcols)
≥ 3	tensor of higher order	$(\text{numdim}_1, \text{numdim}_2, \ldots, \text{numdim}_r)$

- examples:

$$A = \begin{pmatrix} 1.0 & -3.0 & 2.3 & 1.7 \\ 5.6 & 0.0 & -1.3 & 3.4 \\ -7.7 & -3.3 & -2.1 & 5.2 \end{pmatrix}, \quad \text{shape}(A) = (3,4), \quad \text{rank}(A) = 2$$

Computational Graphs

- TensorFlow organizes a computation as a directed graph.
- Nodes represent a tensor.
  - or a list of tensors.
- Tensors can be:
  - stored tensors
    - immutable, value provided at creation time: **tf.constant**
    - immutable, value provided when running the graph: **tf.placeholder**
    - mutable: **tf.Variable**
  - computed tensors (**operations**):
    - having one or more input tensors
    - having one or more output tensors
      – output index: **port**
- Edges represent dependencies.
  - Edge $x \to y$ if y is computed and x one of its inputs.

Sessions

- A session represents the state of an ongoing computation on a computational graph.
- create with default constructor **tf.Session**.
- compute the value of a tensor node with **run**.

Two Phases

1. Construct the Computational Graph
   - create tensor nodes
   - possibly referencing other tensor nodes as inputs
2. Compute values of a node of the Computation Graph (**running**)
   - usually specify target tensor(s)
   - computes all intermediate tensors required for this tensor
   - yield the value of the target tensor(s)

Hello TensorFlow: Add two Constants

```
import tensorflow as tf

a = tf.constant(3.0)
b = tf.constant(4.0)
x = tf.add(a, b)

print(a)
print(b)
print(x)

sess = tf.Session()
x_val = sess.run(x)
print(x_val)
```

Output:

```
Tensor("Const:0", shape=(), dtype=float32)
Tensor("Const_1:0", shape=(), dtype=float32)
Tensor("Add:0", shape=(), dtype=float32)
7
```

Hello TensorFlow: Add two Constants

```python
import tensorflow as tf

a = tf.constant([3.0, -2.7, 1.2])
b = tf.constant([4.0, 5.1, -1.7])
x = tf.add(a, b)

print(a)
print(b)
print(x)

sess = tf.Session()
x_val = sess.run(x)
print(x_val)
```

Output:

```
Tensor("Const_2:0", shape=(3,), dtype=float32)
Tensor("Const_3:0", shape=(3,), dtype=float32)
Tensor("Add_1:0", shape=(3,), dtype=float32)
[ 7.0   2.4   -0.5 ]
```

Tensor Types

- Different element types are represented by tf.DType:

dtype	description
tf.float16	16-bit half-precision floating-point
tf.float32	32-bit single-precision floating-point
tf.float64	64-bit double-precision floating-point
tf.bfloat16	16-bit truncated floating-point
tf.complex64	64-bit single-precision complex
tf.complex128	128-bit double-precision complex
tf.int8	8-bit signed integer
tf.uint8	8-bit unsigned integer
tf.uint16	16-bit unsigned integer
tf.int16	16-bit signed integer
tf.int32	32-bit signed integer
tf.int64	64-bit signed integer
tf.bool	Boolean
tf.string	String
tf.qint8	Quantized 8-bit signed integer
tf.quint8	Quantized 8-bit unsigned integer
tf.qint16	Quantized 16-bit signed integer
tf.quint16	Quantized 16-bit unsigned integer
tf.qint32	Quantized 32-bit signed integer
tf.resource	Handle to a mutable resource

- if omitted, inferred from values:

```
a = tf.constant(4.0)
b = tf.constant(4)
print(a)
print(b)
```

Output:

```
Tensor("Const:0", shape=(), dtype=float32)
Tensor("Const_1:0", shape=(), dtype=int32)
```

Operations: Overloaded Operators

```
import tensorflow as tf

a = tf.constant(3.0)
b = tf.constant(4.0)
x = a + b

print(x)

sess = tf.Session()
x_val = sess.run(x)
print(x_val)
```

Output:

```
Tensor("add_1:0", shape=(), dtype=float32)
7
```

operator	operation node
+	tf.add
-	tf.subtract
*	tf.multiply
/	tf.divide

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$$v = \text{tf.Variable}(\text{initial\_value} = \text{None}, \ldots, \text{name} = \text{None}, \ldots, \text{dtype} = \text{None})$$

- has immutable element type
- has mutable shape (**set_shape**).
- has mutable element values.
  - set by **tf.assign**, **tf.assign_add** (operations)
  - separate values in each session
- has to be initialized before first use:
  - run **v.initializer** operation or
  - run initializers of all variables:

```
init = tf.global_variables_initializer()
sess.run(init)
```

Variables

```python
import tensorflow as tf

x = tf.Variable(3.0)
sess = tf.Session()
sess.run( x.initializer )
x_val = sess.run(x)
print(x_val)

x_plus_one = tf.assign_add(x, 1.0)

for t in range(5):
    x_val = sess.run(x_plus_one)
    print(t, x_val)
```

Output:

```
3.0

0 4.0
1 5.0
2 6.0
3 7.0
4 8.0
```

Initializing from Other Variables

```
import tensorflow as tf

x = tf.Variable(3.0)
y = tf.Variable( tf.multiply(tf.constant(2.0),
                             x.initialized_value()) )
init = tf.global_variables_initializer()
sess = tf.Session()
sess.run(init)
y_val = sess.run(y)
print(y_val)
```

Output:

```
6.0
```

- v.initialized_value assures that a variable has been initialized before
  - do not use

    ```
    y = tf.Variable( tf.multiply(tf.constant(2.0), x) )
    ```

    as x may be selected to be initialized after y.

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Example: Linear Regression

$$\hat{y} := \beta_0 + X\beta \qquad \text{prediction}$$

$$r := y - \hat{y} \qquad \text{residuum}$$

$$\ell := \frac{1}{2}\sum_{n=1}^{N} r_n^2 \qquad \text{loss/error}$$

$$-\frac{\partial \ell}{\partial \beta} := X^T r \qquad \text{negative gradient w.r.t. } \beta$$

$$-\frac{\partial \ell}{\partial \beta_0} := \sum_{n=1}^{N} r_n \qquad \text{negative gradient w.r.t. } \beta_0$$

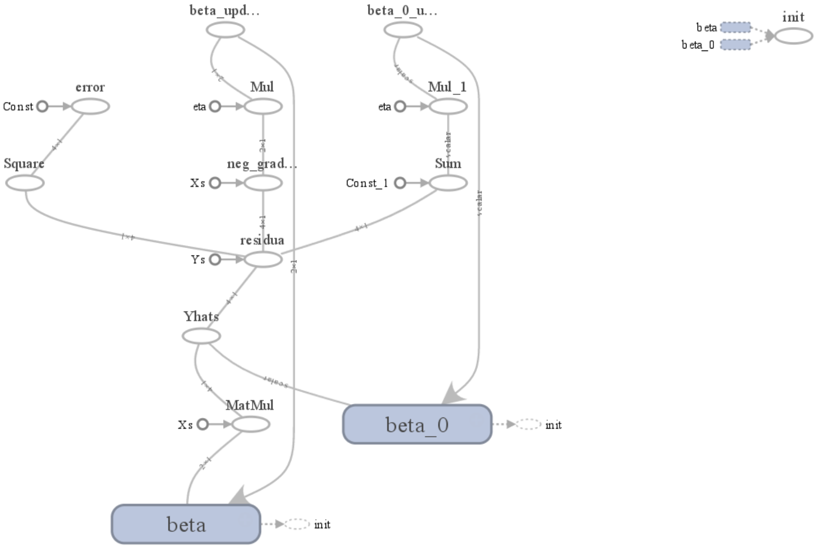
$$\beta^{\text{next}} := \beta - \eta \frac{\partial \ell}{\partial \beta} \qquad \text{update of } \beta$$

$$\beta_0^{\text{next}} := \beta_0 - \eta \frac{\partial \ell}{\partial \beta_0} \qquad \text{update of } \beta_0$$

Example: Linear Regression

```
import tensorflow as tf

Xs_data = [[2,1], [1,2], [4,3], [3,4]]
Ys_data = [[+1], [+1], [-1], [-1]]
eta_data = 0.01

Xs = tf.constant(Xs_data, dtype=tf.float32)
Ys = tf.constant(Ys_data, dtype=tf.float32)
eta = tf.constant(eta_data)

beta = tf.Variable([[0], [0]], dtype=tf.float32)
beta_0 = tf.Variable(0, dtype=tf.float32)

Yhats = tf.add(beta_0, tf.matmul(Xs, beta))
residua = tf.subtract(Ys, Yhats)
error = tf.reduce_sum(tf.square(residua))

neg_grad_beta = tf.matmul(Xs, residua, adjoint_a=True)
beta_update = tf.assign_add(beta, tf.multiply(eta, neg_grad_beta))
beta_0_update = tf.assign_add(beta_0, tf.multiply(eta, tf.reduce_sum(residua)))

init = tf.global_variables_initializer()
sess = tf.Session()
sess.run( init )

for t in range(100):
    error_val, beta_val, beta_0_val = sess.run([error,beta_update,beta_0_update])
    print(t, error_val, beta_0_val, beta_val[0,0], beta_val[1,0])
```

Example: Linear Regression / Computational Graph



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$$\text{tf.gradients}(\text{ys}, \text{xs}, \ldots)$$

- create operations whose final node computes all the gradients

$$\left(\frac{\partial y_n}{\partial x_m}\right)_{n=1,\ldots,N, m=1,\ldots,M} \qquad \text{ys} = (y_1, \ldots, y_N), \text{xs} = (x_1, \ldots, x_M)$$

Example: Linear Regression w. Automatic Gradients

```
import tensorflow as tf

Xs_data = [[2,1], [1,2], [4,3], [3,4]]
Ys_data = [[+1], [+1], [-1], [-1]]
eta_data = 0.01

Xs = tf.constant(Xs_data, dtype=tf.float32)
Ys = tf.constant(Ys_data, dtype=tf.float32)
eta = tf.constant(eta_data)

beta = tf.Variable([[0], [0]], dtype=tf.float32)
beta_0 = tf.Variable(0, dtype=tf.float32)

Yhats = tf.add(beta_0, tf.matmul(Xs, beta))
error = tf.reduce_sum(tf.square(tf.subtract(Ys, Yhats)))

grads = tf.gradients(error, [beta, beta_0])
beta_update = tf.assign_sub(beta, tf.multiply(eta, grads[0]))
beta_0_update = tf.assign_sub(beta_0, tf.multiply(eta, grads[1]))

init = tf.global_variables_initializer()
sess = tf.Session()
sess.run( init )

for t in range(100):
    error_val, beta_val, beta_0_val = sess.run([error,beta_update,beta_0_update])
    print(t, error_val, beta_0_val, beta_val[0,0], beta_val[1,0])
```

How do Automatic Gradients Work?

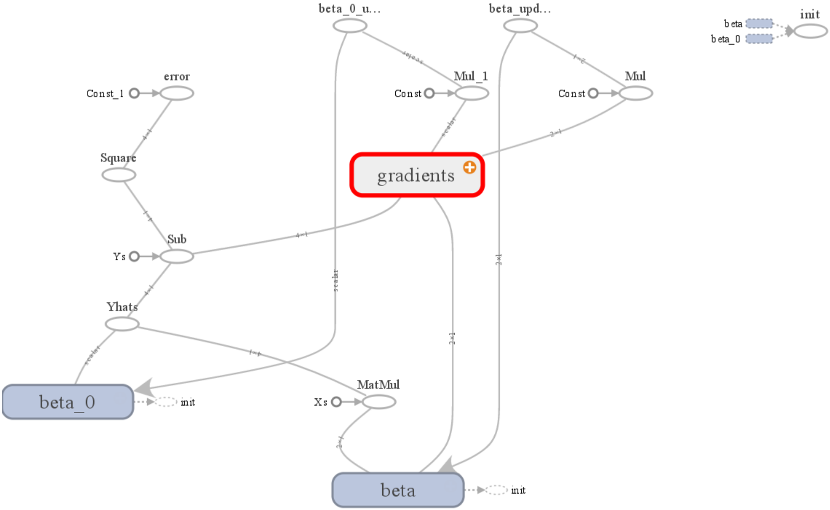
to compute $\frac{\partial y}{\partial x}$:

- find all paths $p^1, \ldots, p^K \in G^*$ in the graph G from x to y
- use chain rule:

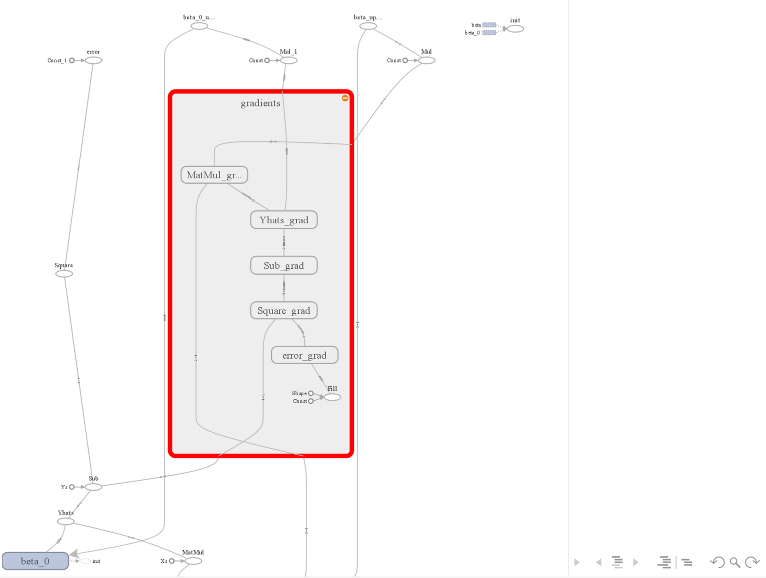
$$\frac{\partial y}{\partial x} = \sum_{k=1}^{K} \prod_{l=|p^k|}^{2} \frac{\partial p_l^k}{\partial p_{l-1}^k}$$

- each operation $p_l^k =: o$ has to provide its gradient $\frac{\partial o}{\partial i}$ for each of its inputs i.
  - then $\frac{\partial \boldsymbol{p_l^k}}{\partial \boldsymbol{p_{l-1}^k}} = \frac{\partial o}{\partial i}$ for $i = p_{l-1}^k$.

Example: LinReg w. Auto Grads / Computational Graph



Example: LinReg w. Auto Grads / Computational Graph



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- representing large data as a whole as a constant is not so useful
  - e.g., if its size exceeds GPU memory, it cannot be deployed to GPU at all.
- better break data into smaller pieces
  - e.g., single instances or minibatches
  - batch GD $\rightarrow$ SGD
- build a graph for a single instance / minibatch
- create placeholder nodes for the instance / minibatch
- placeholders are filled with the **feed_dict** parameter of **run**.

Placeholder Nodes and Feeding

```
import tensorflow as tf

a = tf.placeholder(shape=(), dtype=tf.float32)
b = tf.placeholder(shape=(), dtype=tf.float32)
x = a + b

sess = tf.Session()
print( sess.run(x, {a: 3, b: 7}) )
print( sess.run(x, {a: -2, b: 4}) )
```

Output:

```
10.0
2.0
```

Example: Feeding SGD

```
import tensorflow as tf

Xs_data = [[2,1], [1,2], [4,3], [3,4]]
Ys_data = [+1, +1, -1, -1]
eta_data = 0.01

X = tf.placeholder(shape=(2), dtype=tf.float32)
Y = tf.placeholder(shape=(), dtype=tf.float32)
eta = tf.constant(eta_data)

beta = tf.Variable([0, 0], dtype=tf.float32)
beta_0 = tf.Variable(0, dtype=tf.float32)

Yhat = tf.add(beta_0, tf.reduce_sum(tf.multiply(X, beta)))
error = tf.reduce_sum(tf.square(tf.subtract(Y, Yhat)))

grads = tf.gradients(error, [beta, beta_0])
beta_update = tf.assign_sub(beta, tf.multiply(eta, grads[0]))
beta_0_update = tf.assign_sub(beta_0, tf.multiply(eta, grads[1]))

init = tf.global_variables_initializer()
sess = tf.Session()
sess.run( init )

for t in range(100):
    error_epoch = 0
    for X_data, Y_data in zip(Xs_data, Ys_data):
        error_val, beta_val, beta_0_val = sess.run([error,beta_update,beta_0_update],
                                          { X: X_data, Y: Y_data })
        error_epoch += error_val
    print(t, error_epoch, beta_0_val, beta_val[0], beta_val[1])
```

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Reader Node

```
import tensorflow as tf

data_files = ['lr-data.csv']; eta_data = 0.01

filename_queue = tf.train.string_input_producer(data_files)
reader = tf.TextLineReader(skip_header_lines=1)
_, line = reader.read(filename_queue)

sess = tf.Session()
coord = tf.train.Coordinator()
threads = tf.train.start_queue_runners(coord=coord, sess=sess)

for t in range(6):
    line_val = sess.run(line)
    print(t, line_val)

coord.request_stop()
coord.join(threads)
```

file lr-data.csv:

```
X1, X2, Y
2, 1, +1
1, 2, +1
4, 3, -1
3, 4, -1
```

Output:

```
0 b'2,␣1,␣+1'
1 b'1,␣2,␣+1'
2 b'4,␣3,␣-1'
3 b'3,␣4,␣-1'
4 b'2,␣1,␣+1'
5 b'1,␣2,␣+1'
```

Example: SGD Reading On The Fly

```
import tensorflow as tf
data_files = ['lr-data.csv']; eta_data = 0.01

filename_queue = tf.train.string_input_producer(data_files)
reader = tf.TextLineReader(skip_header_lines=1)
key, value = reader.read(filename_queue)
X1, X2, Y = tf.decode_csv(value, record_defaults=[[0.0],[0.0],[0.0]])
X = tf.stack([X1, X2])
eta = tf.constant(eta_data)

beta = tf.Variable([0, 0], dtype=tf.float32)
beta_0 = tf.Variable(0, dtype=tf.float32)
Yhat = tf.add(beta_0, tf.reduce_sum(tf.multiply(X, beta)))
error = tf.reduce_sum(tf.square(tf.subtract(Y, Yhat)))
grads = tf.gradients(error, [beta, beta_0])
beta_update = tf.assign_sub(beta, tf.multiply(eta, grads[0]))
beta_0_update = tf.assign_sub(beta_0, tf.multiply(eta, grads[1]))
init = tf.global_variables_initializer()
sess = tf.Session() ; sess.run( init )
coord = tf.train.Coordinator()
threads = tf.train.start_queue_runners(coord=coord, sess=sess)

error_epoch = 0
for t in range(400):
    error_val, beta_val, beta_0_val = sess.run([error,beta_update,beta_0_update])
    error_epoch += error_val
    if t % 10 == 0:
        print(t, error_epoch, beta_0_val, beta_val[0], beta_val[1])
        error_epoch = 0
coord.request_stop()
coord.join(threads)
```

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Debugging: Visualize Computational Graph

1. Create a summary.FileWriter for the session and graph before running the session:

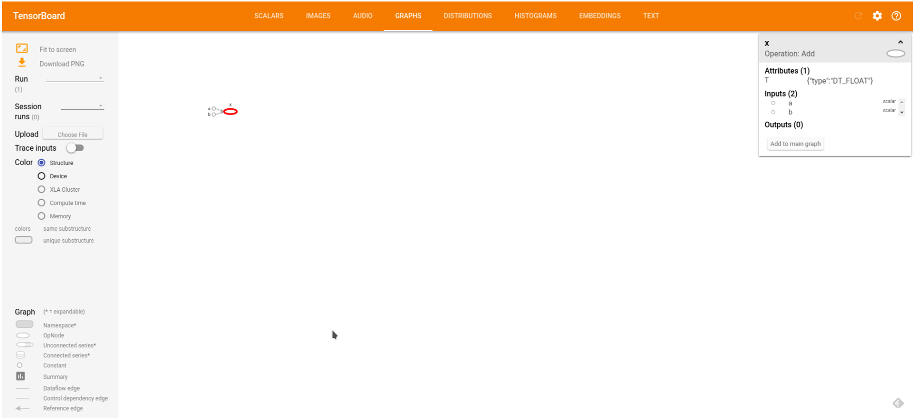
```
import tensorflow as tf

a = tf.constant(3.0, name='a')
b = tf.constant(4.0, name='b')
x = tf.add(a, b, name='x')

print(a)

sess = tf.Session()
log = tf.summary.FileWriter('logs/add-two-constants.log', sess.graph)
x_val = sess.run(x)
log.close()
print(x_val)
```

2. run tensorboard on the logdir:

```
> tensorboard --logdir logs/add-two-constants.log
```

3. open localhost:6006 in your browser

Debugging: Visualize Computational Graph



Summary (1/3)

- TensorFlow represents computations as **graphs**.
  - nodes representing (a list of) **tensors**.
    - stored:
      — immutable: **constant**, **placeholder**
      — mutable: **variable**
    - computed: **operation**
  - edges representing dependencies
    - $x \rightarrow y$: y is computed and x is one of its inputs
- Two phases:
  - graph construction
  - executing (parts of) the graph (**running**)

Summary (2/3)

- Nodes can be **distributed over different devices**.
  - cores of a CPU, GPUs, different compute nodes
  - **automatic placement** based on cost heuristics
    - eligible: sufficient memory available
    - expected runtime
      — based on cost heuristics
      — possibly also based on past runs
    - expected time for data movement between devices
- Operations can be assembled from dozens of **elementary operations**.
  - elementary math: add, subtract, multiply, divide
  - elementwise functions: log, exp, etc.
  - matrix operations: matrix product, inversion, etc.
  - structual tensor operations: slicing, stacking etc.

Summary (3/3)

- **Gradients** can be computed automatically.
  - simply using the chain rule
  - and explicit gradients for all elementary operations.
  - gradients add nodes to the graph.
- Medium-sized data should be broken into parts and **fed into a placeholder** for parts
  - e.g., SGD: single instances or minibatches
  - medium-sized data:
    - too large for the GPU
    - still can be read on a single data node
- Large data must be read by **reader nodes** as part of the graph execution.
  - large data: must be read on different data nodes in a distributed fashion

Further Readings

- TensorFlow white paper:
  - Abadi et al. [2016]
  - not yet fully complete: evaluation section is missing

References I

Martín Abadi, Ashish Agarwal, Paul Barham, Eugene Brevdo, Zhifeng Chen, Craig Citro, Greg S Corrado, Andy Davis, Jeffrey Dean, Matthieu Devin, et al. Tensorflow: Large-scale machine learning on heterogeneous distributed systems. *arXiv preprint arXiv:1603.04467*, 2016.