Differentiable Learning of Logical Rules for Knowledge Base Reasoning

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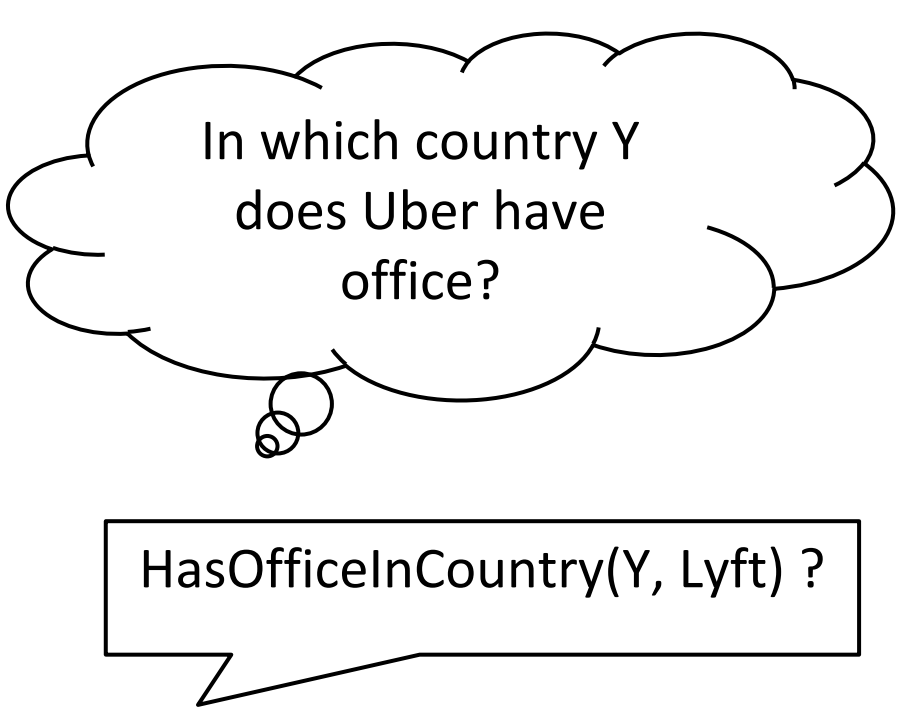
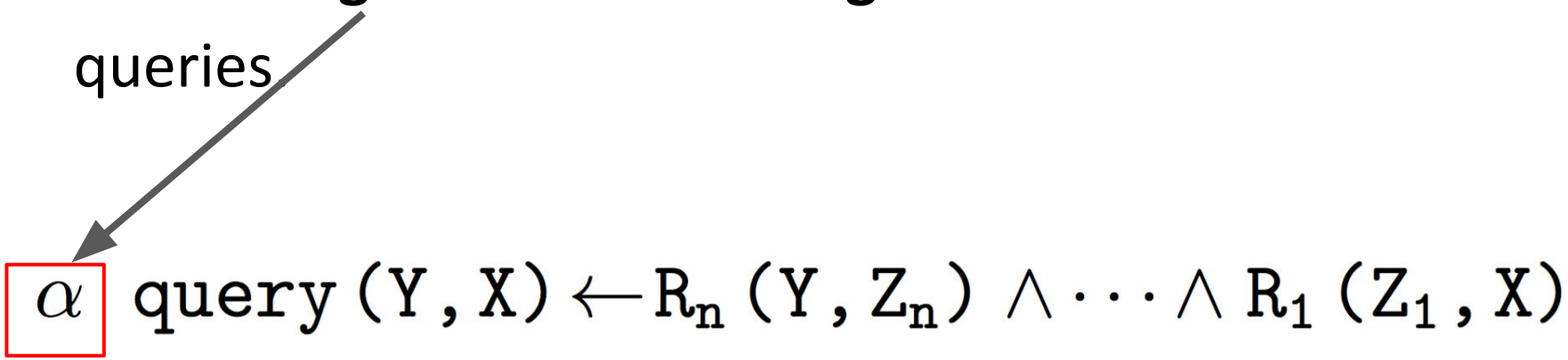
Problem definition

- Knowledge base (KB) reasoning
  - KB: a set of binary relations between entities.
  - Reasoning: retrieve entities from KB based on queries.



Our approach

- Learn **weighted chain-like logical rules** to answer queries



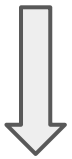
0.7 HasOfficeInCountry (Y, X) ← CityInCountry(Y, W) ⋀ HasOfficeInCity(W, X)

ungrounded variables

TensorLog Operators

- Represent **logical rule inference** using TensorLog operators (i.e. sparse matrices).
  - E = set of entities. R = set of binary relations.
  - For each entity i, define one-hot vector v_i.
  - For each relation R, define adjacency matrix M_R.

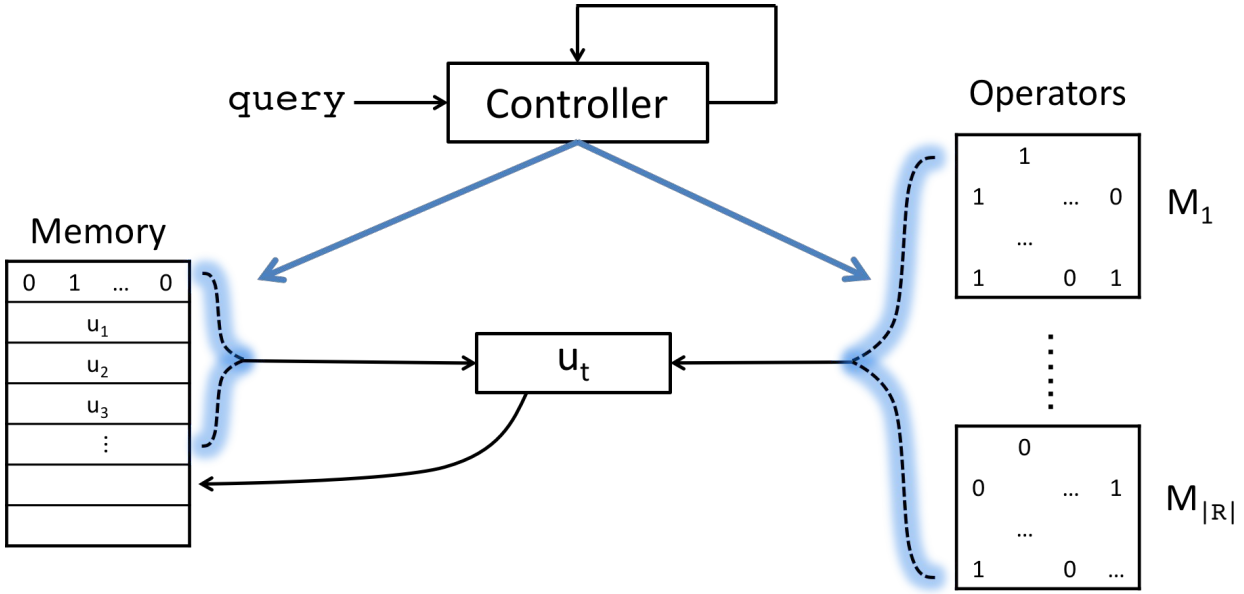
0.7 HasOfficeInCountry (Y, x) ← CityInCountry(Y, W) ⋀ HasOfficeInCity(W, x)



$$v_y = 0.7\ M_{\text{CityInCountry}}\ M_{\text{HasOfficeInCity}}\ v_x$$

Learn the logical rules

- Equivalent to **learning to compose** the operators.



$$\mathbf{u_0} = \mathbf{v_x}$$

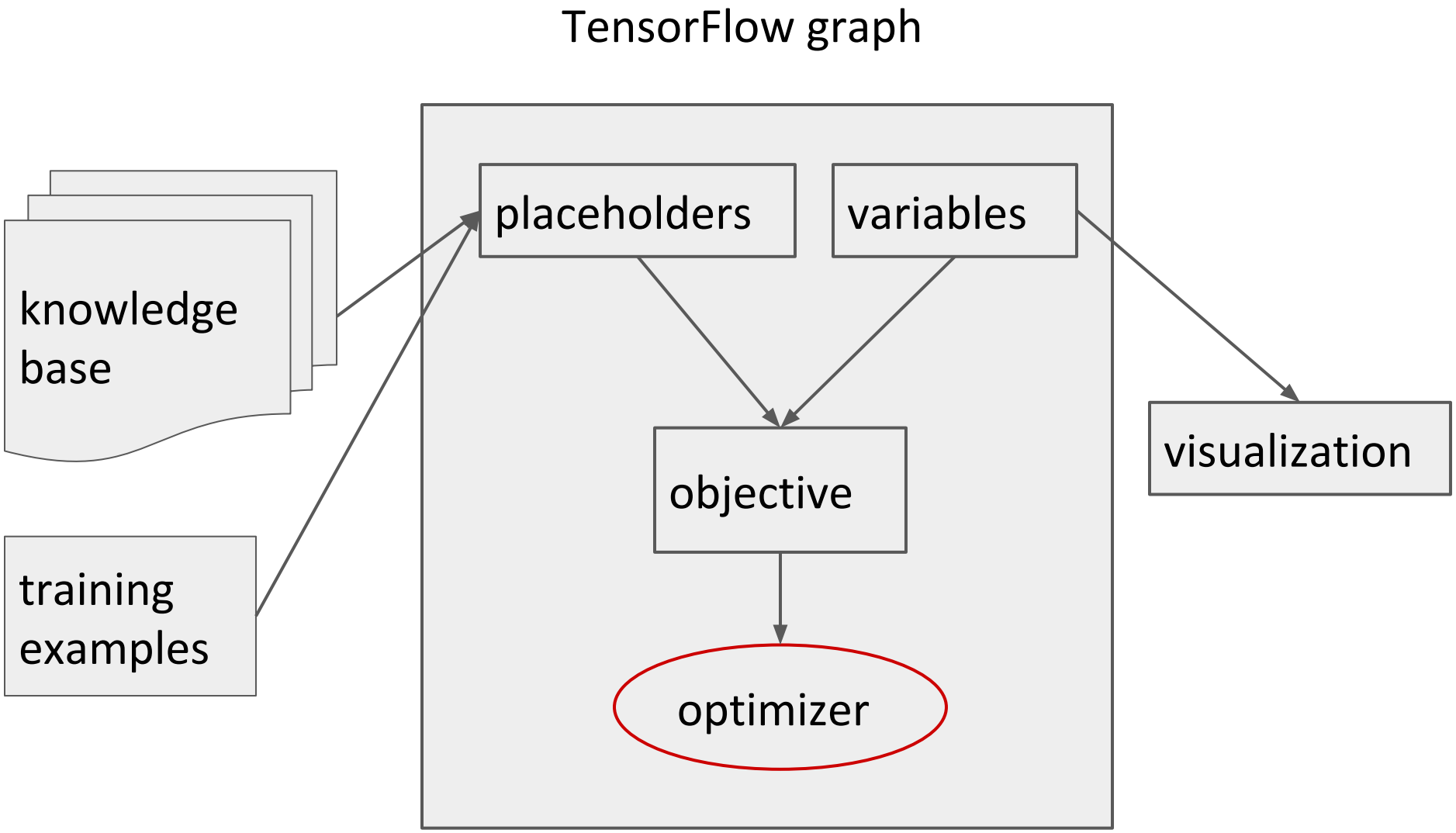
$$\mathbf{u_t} = \sum_{\mathbf{k}}^{|\mathbf{R}|} a_t^{\mathbf{k}} \mathbf{M}_{\mathbf{R_k}} \left(\sum_{\tau=0}^{t-1} b_t^{\tau} \mathbf{u}_{\tau} \right) \quad \text{for } 1 \leq t \leq T$$

$$\mathbf{u_{T+1}} = \sum_{\tau=0}^{T} b_{T+1}^{\tau} \mathbf{u}_{\tau}$$

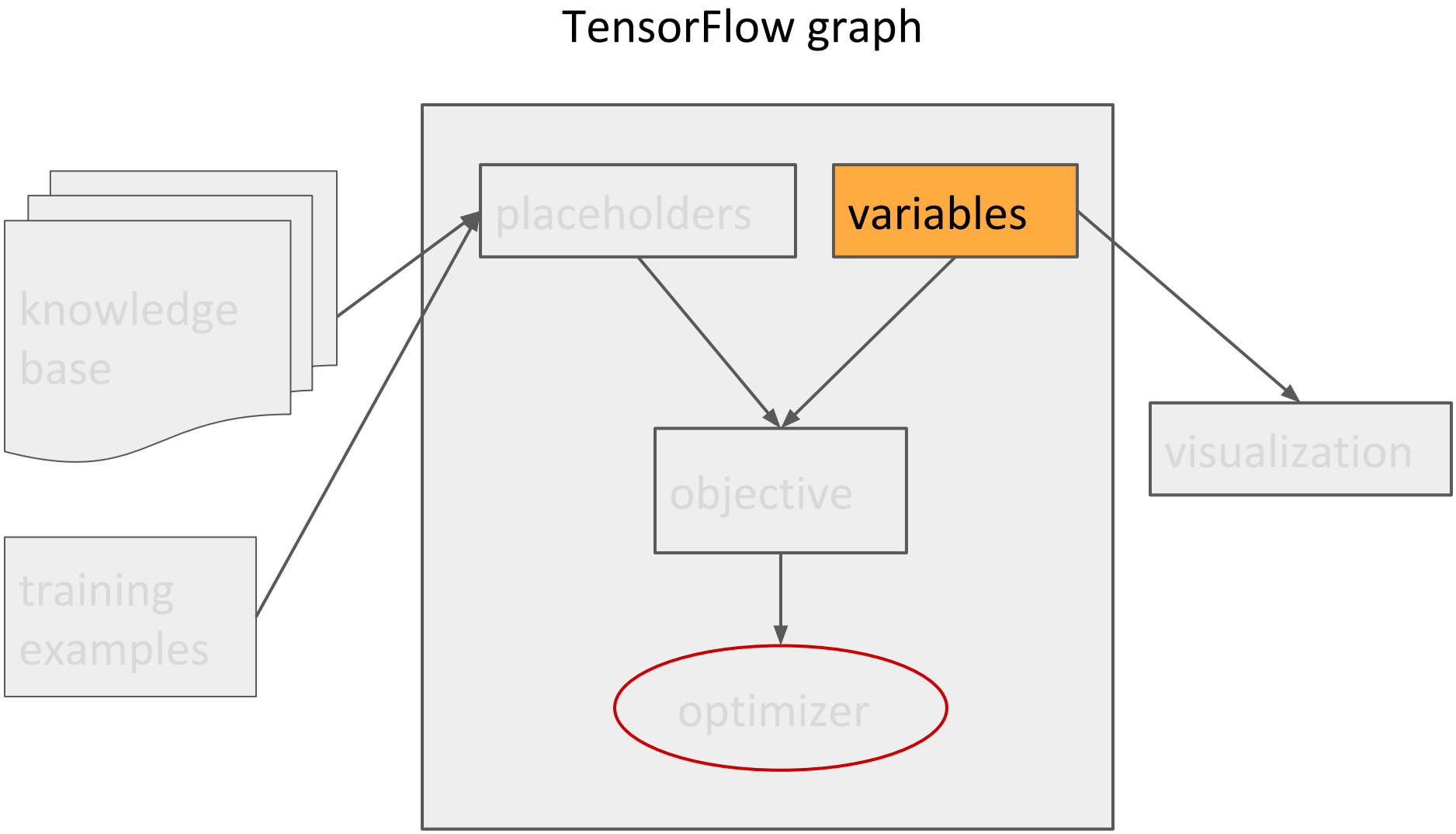
Implementation Outline

- Overview
- Learnable parameters
- Data flow and representation
- Training
- Sidelines for visualization

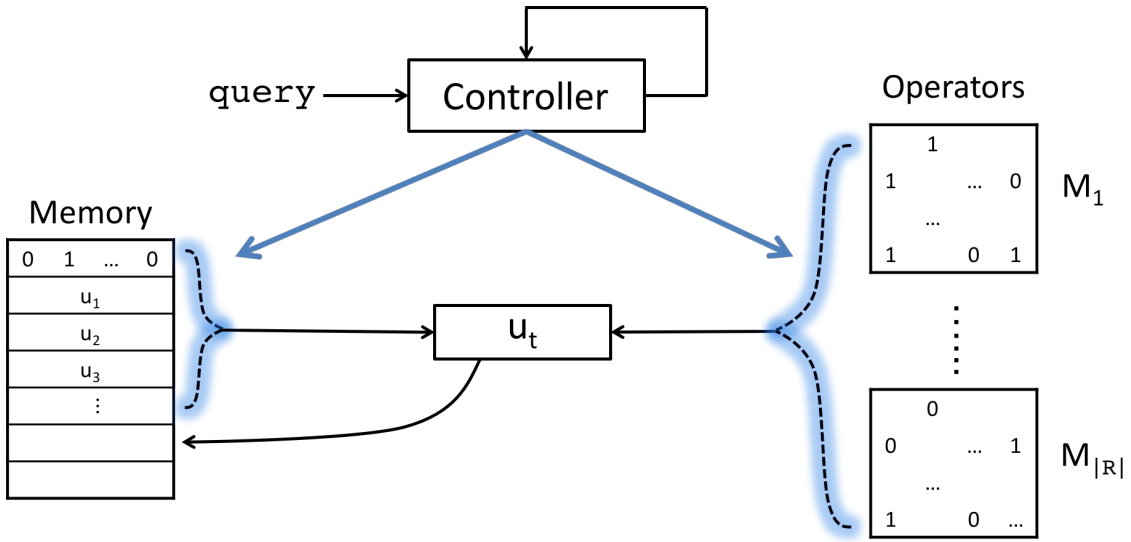
Implementation overview



Learnable parameters



Learnable parameters



Embeddings

RNN cell

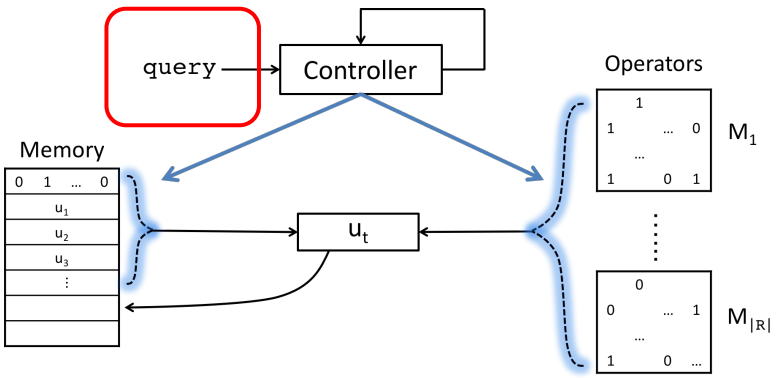
A linear layer

$$\mathbf{h_t} = \text{update}\left(\mathbf{h_{t-1}}, \text{input}\right)$$

$$\mathbf{a_t} = \text{softmax}\left(W\mathbf{h_t} + b\right)$$

$$\mathbf{b_t} = \text{softmax}\left(\left[\mathbf{h_0}, \ldots, \mathbf{h_{t-1}}\right]^T \mathbf{h_t}\right)$$

Implementing the architecture 1/5



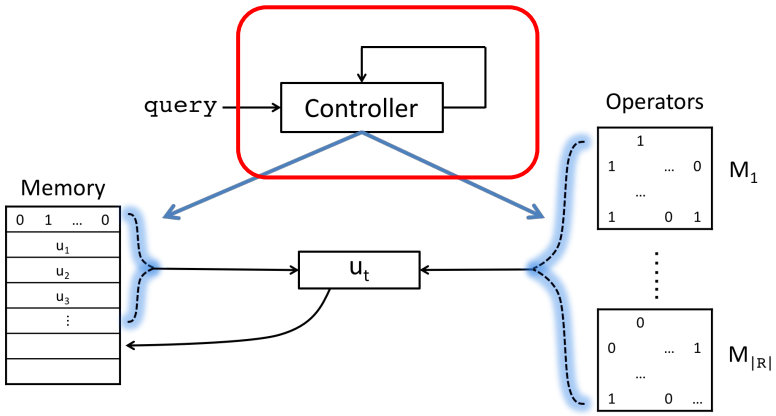

```
if not self.query_is_language:
    self.queries = tf.placeholder(tf.int32, [None, self.num_step])
    self.query_embedding_params = tf.Variable(self._random_uniform_unit(
                                                self.num_query + 1, # <END> token
                                                self.query_embed_size),
                                              dtype=tf.float32)

    rnn_inputs = tf.nn.embedding_lookup(self.query_embedding_params,
                                        self.queries)
else:
    self.queries = tf.placeholder(tf.int32, [None, self.num_step, self.num_word])
    self.vocab_embedding_params = tf.Variable(self._random_uniform_unit(
                                                self.num_vocab + 1, # <END> token
                                                self.vocab_embed_size),
                                              dtype=tf.float32)
    embedded_query = tf.nn.embedding_lookup(self.vocab_embedding_params,
                                            self.queries)
    rnn_inputs = tf.reduce_mean(embedded_query, axis=2)

return rnn_inputs
```

- Query format
  - Natural language
  - Structured

Implementing the architecture 2/5



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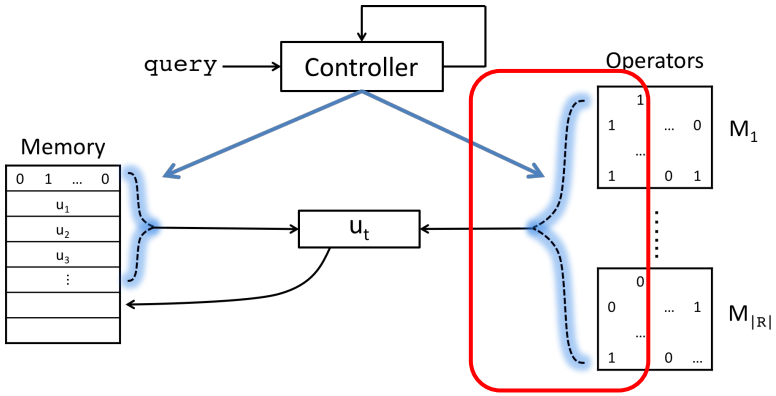
```
""" Build a computation graph that represents the model """
rnn_inputs = self._build_input()
# rnn_inputs: a list of num_step tensors,
# each tensor of size (batch_size, query_embed_size).
self.rnn_inputs = [tf.reshape(q, [-1, self.query_embed_size])
                   for q in tf.split(rnn_inputs,
                                     self.num_step,
                                     axis=1)]

cell = tf.contrib.rnn.core_rnn_cell.LSTMCell(self.rnn_state_size,
                                             state_is_tuple=True)
self.cell = tf.contrib.rnn.core_rnn_cell.MultiRNNCell(
                                             [cell] * self.num_layer,
                                             state_is_tuple=True)
init_state = self.cell.zero_state(tf.shape(self.tails)[0], tf.float32)

# rnn_outputs: a list of num_step tensors,
# each tensor of size (batch_size, rnn_state_size).
self.rnn_outputs, self.final_state = tf.contrib.rnn.static_rnn(
                                        self.cell,
                                        self.rnn_inputs,
                                        initial_state=init_state)
```

Implementing the architecture 3/5



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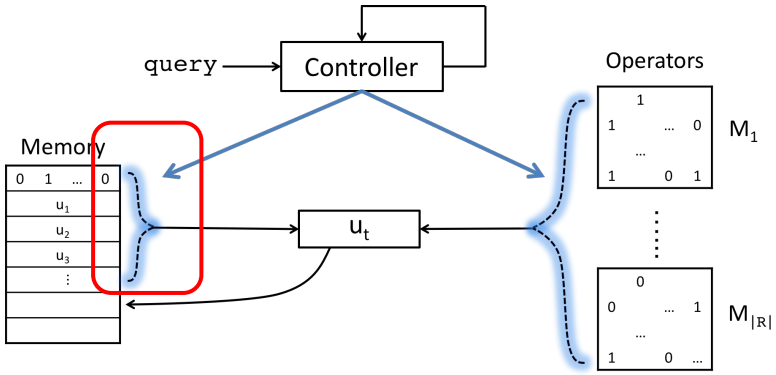
```
self.W = tf.Variable(np.random.randn(
                         self.rnn_state_size,
                         self.num_operator),
                     dtype=tf.float32)
self.b = tf.Variable(np.zeros(
                         (1, self.num_operator)),
                     dtype=tf.float32)

# attention_operators: a list of num_step lists,
# each inner list has num_operator tensors,
# each tensor of size (batch_size, 1).
# Each tensor represents the attention over an operator.
self.attention_operators = [tf.split(
                             tf.nn.softmax(
                               tf.matmul(rnn_output, self.W) + self.b),
                             self.num_operator,
                             axis=1)
                             for rnn_output in self.rnn_outputs]
```

Implementing the architecture 4/5



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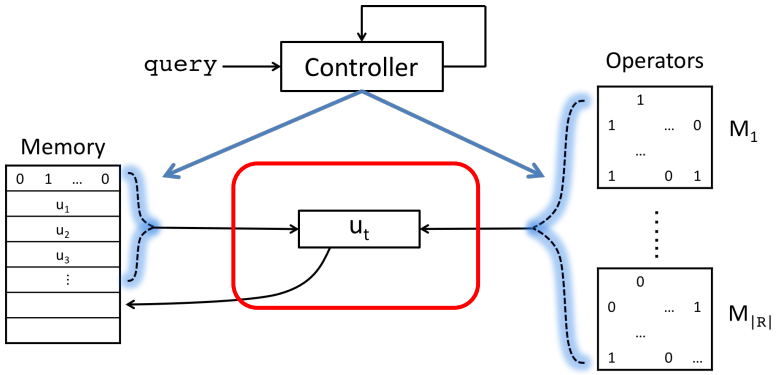
$$\mathbf{b_t} = \text{softmax}\left(\left[\mathbf{h_0}, \ldots, \mathbf{h_{t-1}}\right]^T \mathbf{h_t}\right)$$

```
for t in xrange(self.num_step):
    self.attention_memories.append(
                    tf.nn.softmax(
                    tf.squeeze(
                        tf.matmul(
                            tf.expand_dims(self.rnn_outputs[t], 1),
                            tf.stack(self.rnn_outputs[0:t+1], axis=2)),
                    squeeze_dims=[1])))

    # memory_read: tensor of size (batch_size, num_entity)
    memory_read = tf.squeeze(
                    tf.matmul(
                        tf.expand_dims(self.attention_memories[t], 1),
                        self.memories),
                    squeeze_dims=[1])
```

Implementing the architecture 5/5



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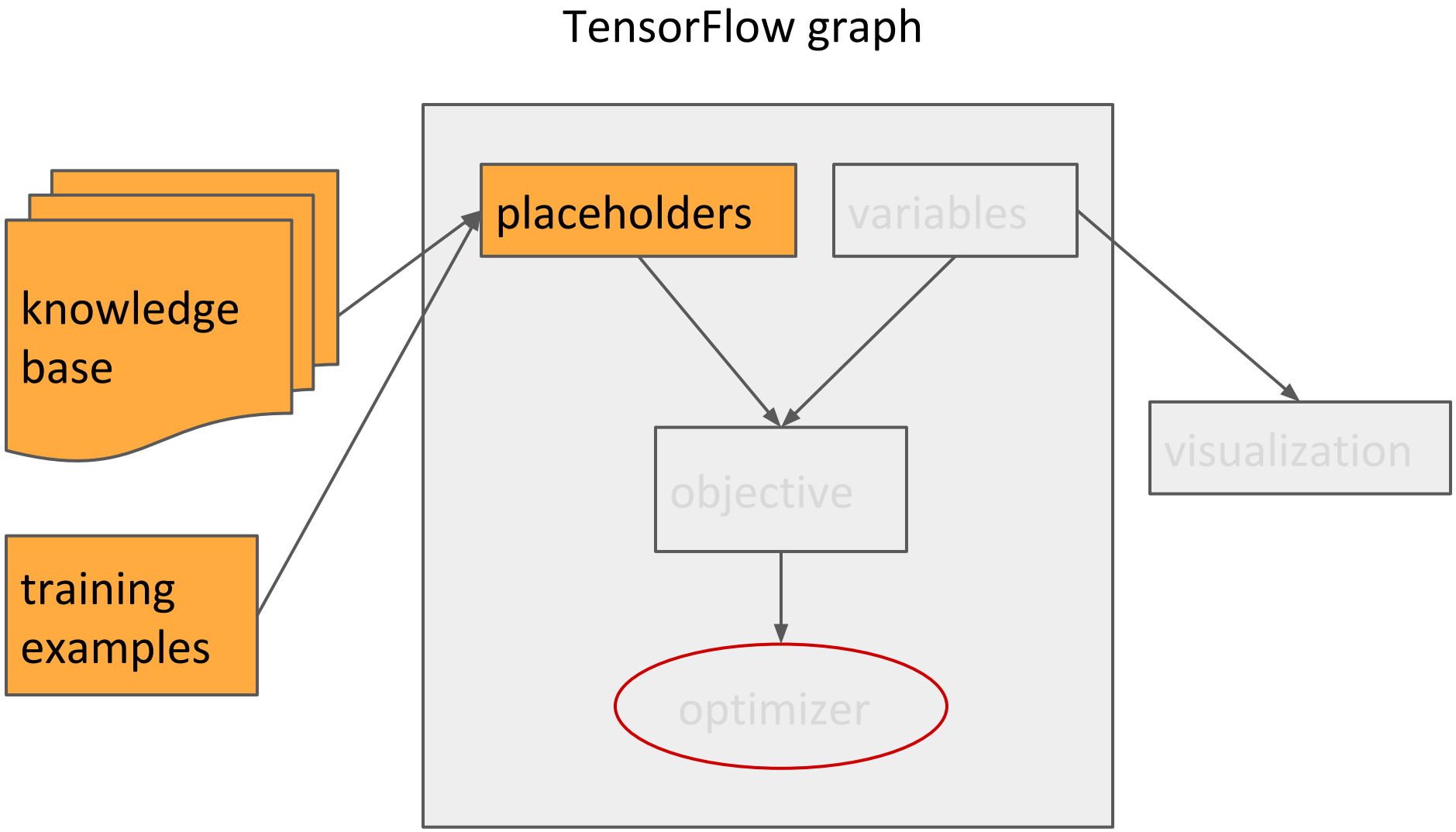
$$\mathbf{u_{T+1}} = \sum_{\tau=0}^{T} b_{T+1}^{\tau} \mathbf{u}_{\tau}$$

```
for r in xrange(self.num_operator/2):
    for op_matrix, op_attn in zip(
                    [self.database[r],
                     tf.sparse_transpose(self.database[r])],
                    [self.attention_operators[t][r],
                     self.attention_operators[t][r+self.num_operator/2]]):
        product = tf.sparse_tensor_dense_matmul(op_matrix, memory_read)
        database_results.append(tf.transpose(product) * op_attn)

added_database_results = tf.add_n(database_results)

# Populate a new cell in memory by concatenating.
self.memories = tf.concat(
    [self.memories,
    tf.expand_dims(added_database_results, 1)],
    axis=1)
```

Data flow


TensorFlow graph
knowledge base
training examples
placeholders
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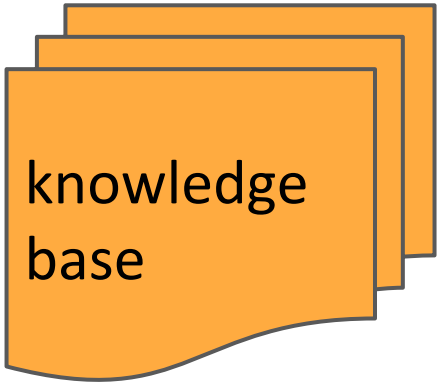
visualization

Data representation



Format:

- e_A Relation e_B

num_operator

num_entity

training
examples

Format:

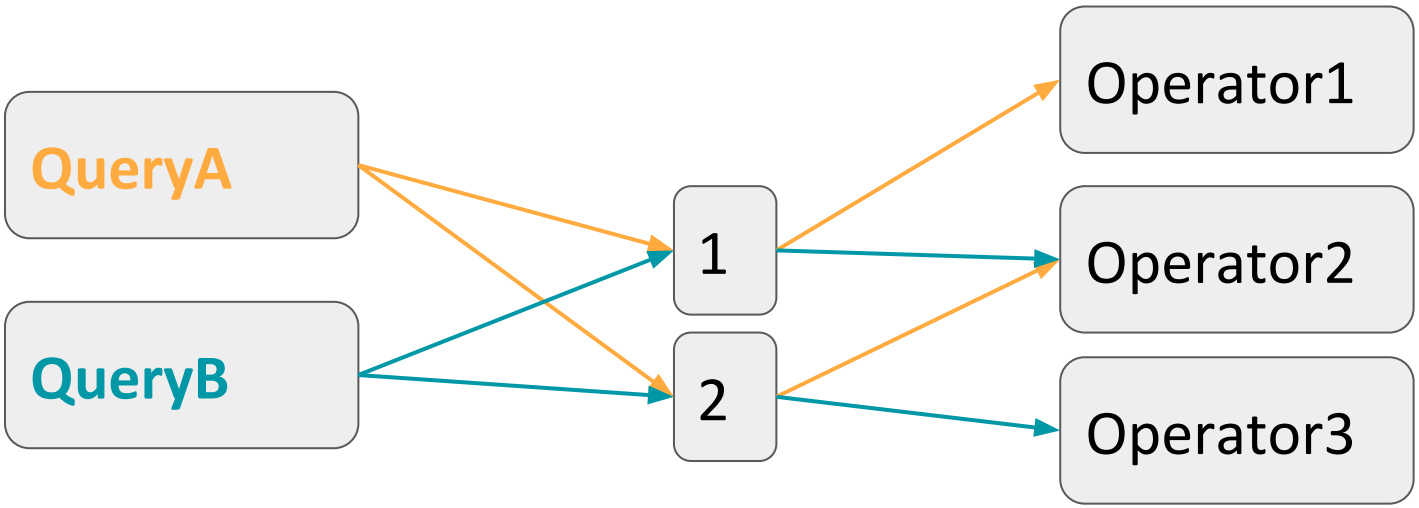
- natural language
  - e_{head}, w_1, …, w_n, e_{tail}
- structured
  - e_{head}, query, e_{tail}

num_vocab

num_query

Data representation

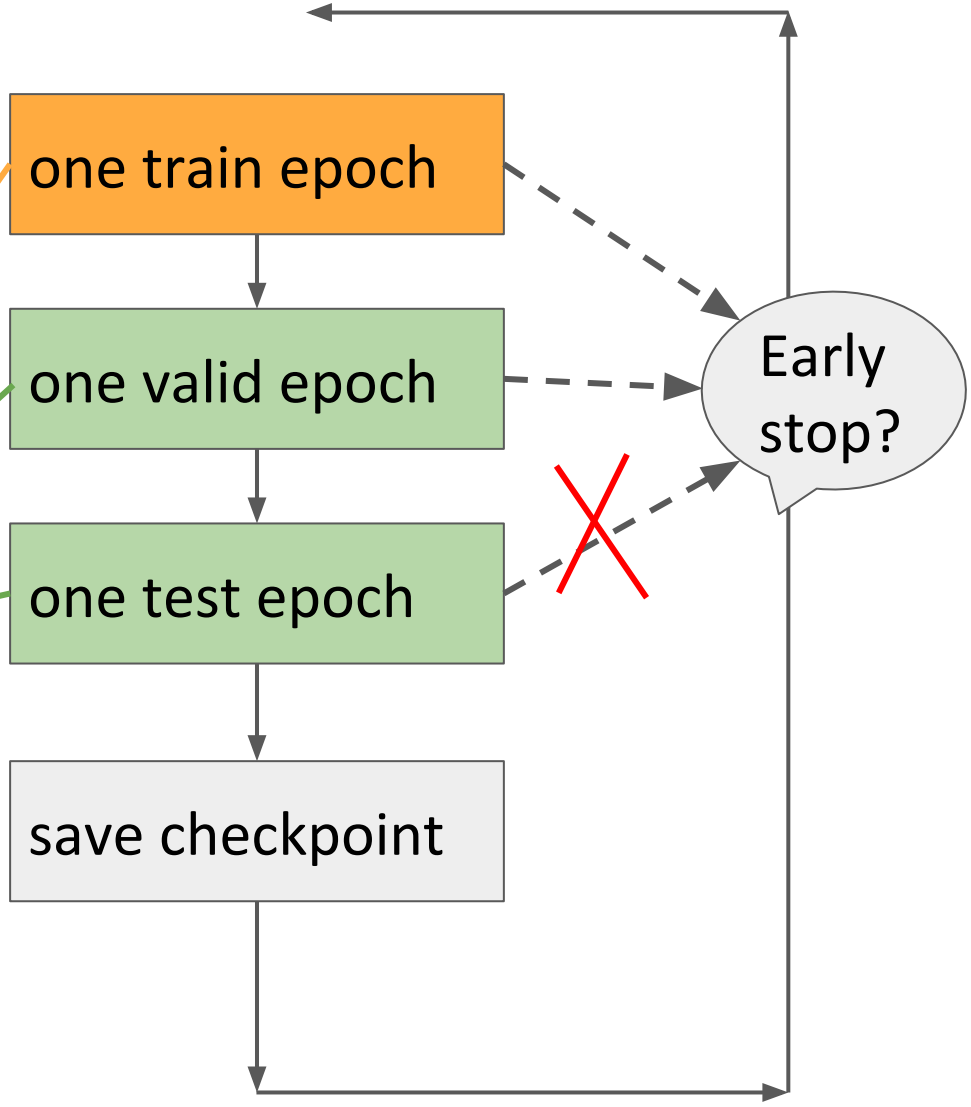
- Mapping
  - query_to_id
    - Used to look up embeddings.
  - id_to_operator
    - Can vary across queries.



Training

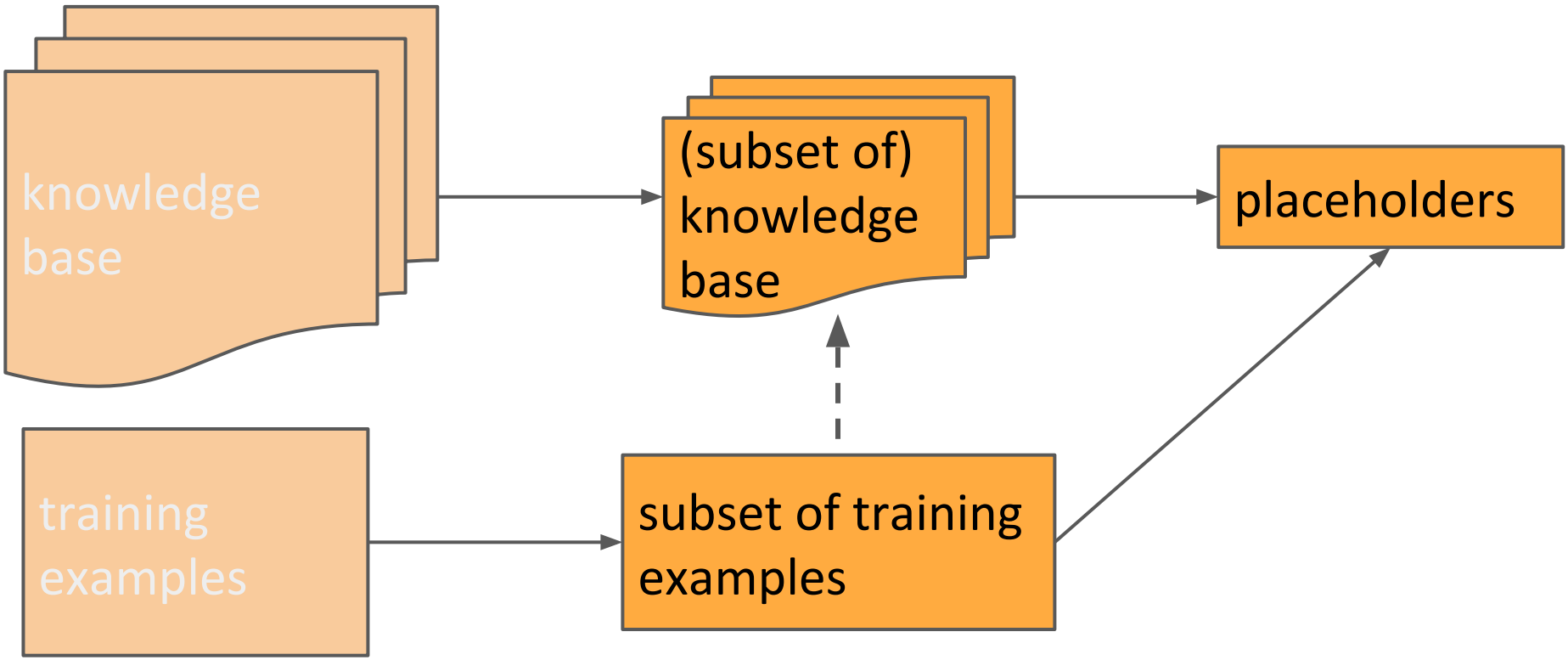
```
def one_epoch(self, mode, num_batch, next_fn):
    epoch_loss = []
    epoch_in_top = []
    for batch in xrange(num_batch):
        if (batch+1) % max(1, (num_batch / self.option.pr
            sys.stdout.write("%d/%d\t" % (batch+1, num_ba
            sys.stdout.flush()

        (qq, hh, tt), mdb = next_fn()
        if mode == "train":
            run_fn = self.learner.update
        else:
            run_fn = self.learner.predict
        loss, in_top = run_fn(self.sess,
                              qq,
                              hh,
                              tt,
                              mdb)
        epoch_loss += list(loss)
        epoch_in_top += list(in_top)
```

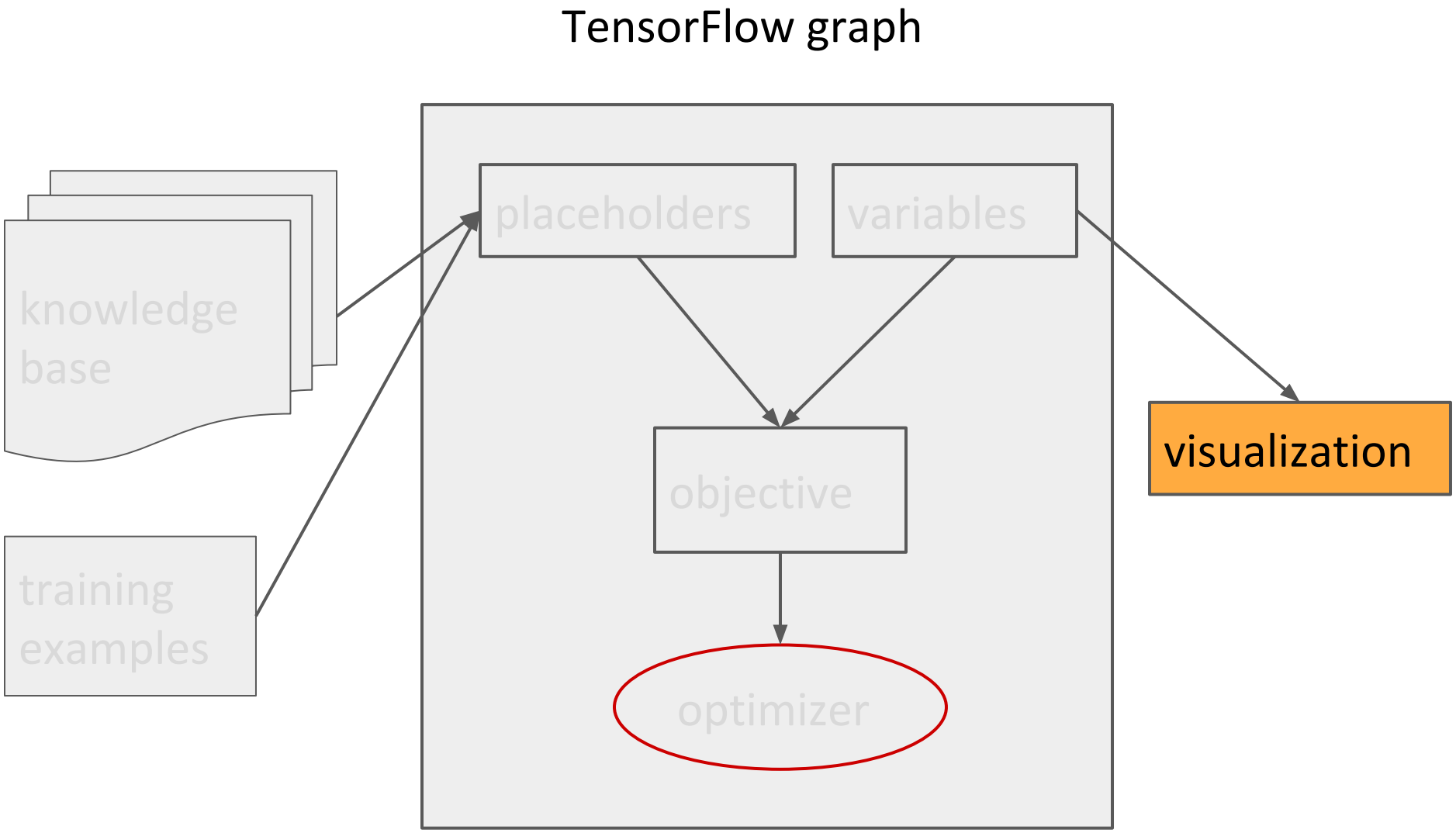


Training

- Batching
  - Batch size depends on how much CPU/GPU memory is available.
  - Examples in the batch use the same knowledge base.



Sidelines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Future work

- Scalability
  - Use graph sampling to reduce num_entity.
- Expressiveness
  - Extend chain-like rules to poly-tree.
- Application
  - Queries in the format of images.

Thanks!

Checkout our implementation at:

https://github.com/fanyangxyz/Neural-LP