Deep Probabilistic Programming with Edward

Dustin Tran†, Matt Hoffman*‡, Kevin Murphy‡, Eugene Brevdo‡, Rif Saurous‡, David Blei†

†Columbia University, *Adobe Research, ‡Google

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Summary

- Deep neural networks are popular in large part due to their compositional nature. How do we do this for probabilistic modeling?
- We describe Edward, a new Turing-complete probabilistic programming language.
- Edward builds two representations—random variables and inference.
- For example, we show how to design rich variational models and generative adversarial networks.

Comopsitional Representations for Probabilistic Models

- We define random variables as the key compositional representation.
- They are class objects e.g. with log-density and sample methods.
- Each random variable $\mathbf{x}$ is associated to a tensor $\mathbf{x}^*$ in the computational graph, which represents a single sample $\mathbf{x}^* \sim p(\mathbf{x})$.
- Mutable states represent enable conditioning sets to vary, $p(\mathbf{y} \mid \mathbf{x})$ and optimization of parameters, $p(\mathbf{x}; \theta)$.

Compositional Representations for Inference

- Given data $\mathbf{x}_{\text{train}}$, inference aims to calculate the posterior $p(\mathbf{z}, \beta \mid \mathbf{x}_{\text{train}}; \boldsymbol{\theta})$, where $\boldsymbol{\theta}$ are any model parameters to estimate.
- In variational inference, the idea is to posit an approximating family $q \in \mathcal{Q}$ and to find the closest member q^*. We write it with mutable states representing its parameters, where $q(\beta; \mu, \sigma) = \text{Normal}(\beta; \mu, \sigma)$, $q(\mathbf{z}; \pi) = \text{Categorical}(\mathbf{z}; \pi)$.

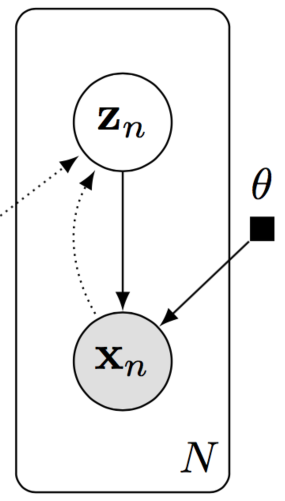
```
qbeta = Normal(mu=tf.Variable(tf.zeros([K, D])),
               sigma=tf.exp(tf.Variable(tf.zeros[K, D])))
qz = Categorical(logits=tf.Variable(tf.zeros[N, K]))

inference = ed.VariationalInference({beta: qbeta, z: qz}, data={x: x_train})
```

- Specific variational algorithms inherit from VariationalInference to define their own methods, e.g., a loss function and gradient.
- Monte Carlo approximates the posterior using samples. We represent it where the approximating family is an empirical distribution, $q(\beta; \{\beta^{(t)}\}) = \frac{1}{T}\sum_{t=1}^{T} \delta(\beta, \beta^{(t)})$, $q(\mathbf{z}; \{\mathbf{z}^{(t)}\}) = \frac{1}{T}\sum_{t=1}^{T} \delta(\mathbf{z}, \mathbf{z}^{(t)})$.

```
T = 10000  # number of samples
qbeta = Empirical(params=tf.Variable(tf.zeros([T, K, D]))
qz = Empirical(params=tf.Variable(tf.zeros([T, N]))

inference = ed.MonteCarlo({beta: qbeta, z: qz}, data={x: x_train})
```

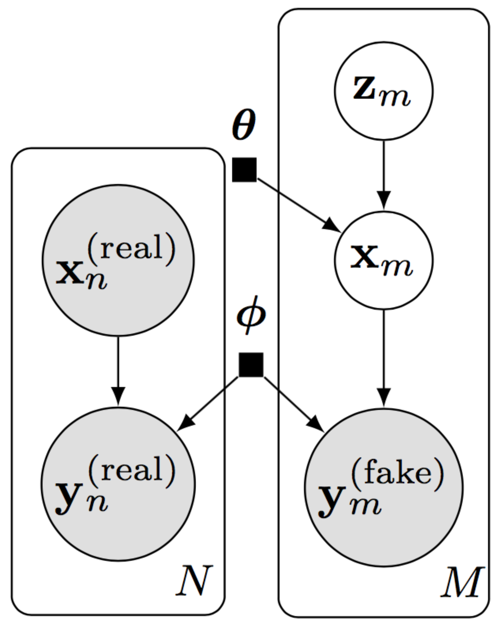
- Monte Carlo algorithms proceed by updating one sample $\beta^{(t)}, \mathbf{z}^{(t)}$ at a time in the empirical approximation. Specific MC samplers determine the update rules.

Example: Variational Auto-Encoder



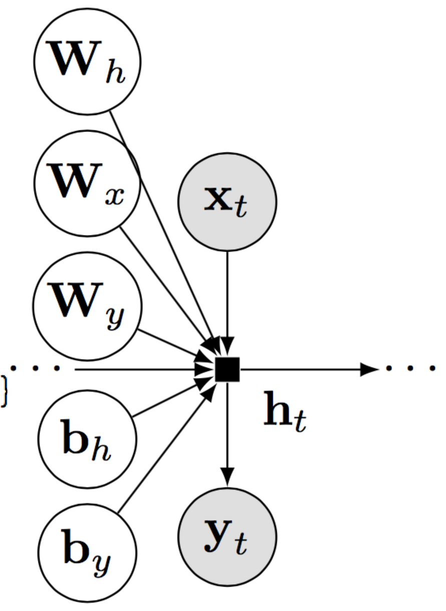

```
# Probabilistic model
z = Normal(mu=tf.zeros([N, d]), sigma=tf.ones([N, d]))
h = slim.fully_connected(z, 256, activation_fn=tf.nn.relu)
x = Bernoulli(logits=slim.fully_connected(h, 28 * 28))

# Variational model
qx = tf.placeholder(tf.float32, [N, 28 * 28])
qh = slim.fully_connected(qx, 256, activation_fn=tf.nn.relu)
qz = Normal(mu=slim.fully_connected(qh, d)
  sigma=slim.fully_connected(qh, d, activation_fn=tf.nn.softplus)
```

Example: Generative Adversarial Networks




```
# Probabilistic model
z = Normal(mu=tf.zeros([M, d]), sigma=tf.ones([M, d]))
x = generative_network(z)

# augmentation for GAN-based inference
y_fake = Bernoulli(logits=discriminative_network(x))
y_real = Bernoulli(logits=discriminative_network(x_real))

data = {y_real: tf.ones(N), y_fake: tf.zeros(M)}
inference = ed.GANInference(data=data)
```

Example: Bayesian RNN with Variable Length




```
def rnn_cell(hprev, xt):
  return tf.tanh(tf.dot(hprev, Wh) + tf.dot(xt, Wx) + bh)

Wh = Normal(mu=tf.zeros([H, H]), sigma=tf.ones([H, H]))
Wx = Normal(mu=tf.zeros([D, H]), sigma=tf.ones([D, H]))
Wy = Normal(mu=tf.zeros([H, 1]), sigma=tf.ones([H, 1]))
bh = Normal(mu=tf.zeros(H), sigma=tf.ones(H))
by = Normal(mu=tf.zeros(1), sigma=tf.ones(1))

x = tf.placeholder(tf.float32, [None, D])
h = tf.scan(rnn_cell, x, initializer=tf.zeros(H))
y = Normal(mu=tf.matmul(h, Wy) + by, sigma=1.0)
```

Composing Inferences

Core to Edward's design is that inference can be written as a collection of separate inference programs. Below we demonstrate variational EM.

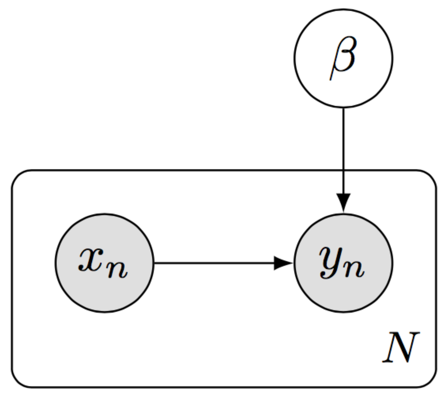
```
qbeta = PointMass(params=tf.Variable(tf.zeros([K, D])))
qz = Categorical(logits=tf.Variable(tf.zeros[N, K]))

inference_e = ed.VariationalInference({z: qz}, data={x: x_data, beta: qbeta})
inference_m = ed.MAP({beta: qbeta}, data={x: x_data, z: qz})

for _ in range(10000):
  inference_e.update()
  inference_m.update()
```

Experiments: Recent Methods in Variational Inference

Inference method	Negative log-likelihood
Variational auto-encoder (VAE) [3]	≤ 88.2
VAE without analytic KL	≤ 89.4
VAE with analytic entropy	≤ 88.1
VAE with score function gradient	≤ 87.9
Normalizing flows [5]	≤ 85.8
Hierarchical variational model [4]	≤ 85.4
Importance-weighted auto-encoders ($K = 50$) [1]	≤ 86.3
HVM with IWAE objective ($K = 5$)	≤ 85.2
Rényi divergence ($\alpha = -1$)	≤ 140.5

Inference methods for a probabilistic decoder on binarized MNIST. The Edward PPL makes it easy to experiment with many algorithms.

Experiments: GPU-accelerated Hamiltonian Monte Carlo




```
# Model
x = tf.Variable(x_data, trainable=False)
beta = Normal(mu=tf.zeros(D), sigma=tf.ones(D))
y = Bernoulli(logits=tf.dot(x, beta))

# Inference
qbeta = Empirical(params=tf.Variable(tf.zeros([T, D])))
inference = ed.HMC({beta: qbeta}, data={y: y_data})
inference.run(step_size=0.5 / N, n_steps=100)
```

We perform inference on Bayesian logistic regression for the Covertype dataset ($N = 581012$, $D = 54$). We use a 12-core Intel i7-5930K CPU at 3.50GHz and a NVIDIA Titan X (Maxwell) GPU.
We compare the runtime of HMC for 100 iterations (and same settings).

Probabilistic programming language	Runtime
Stan (1 CPU) [2]	171 sec
PyMC3 (12 CPU) [6]	361 sec
Edward (12 CPU)	**8.2 sec**
Edward (GPU)	**4.9 sec** (35x faster than Stan)

References

[1] Burda, Y., Grosse, R., and Salakhutdinov, R. (2016). Importance weighted autoencoders. In *International Conference on Learning Representations*.

[2] Carpenter, B., Gelman, A., Hoffman, M. D., Lee, D., Goodrich, B., Betancourt, M., Brubaker, M., Guo, J., Li, P., and Riddell, A. (2016). Stan: A probabilistic programming language. *Journal of Statistical Software*.

[3] Kingma, D. P. and Welling, M. (2014). Auto-encoding variational Bayes. In *International Conference on Learning Representations*.

[4] Ranganath, R., Tran, D., and Blei, D. M. (2016). Hierarchical variational models. In *International Conference on Machine Learning*.

[5] Rezende, D. J. and Mohamed, S. (2015). Variational inference with normalizing flows. In *International Conference on Machine Learning*.

[6] Salvatier, J., Wiecki, T., and Fonnesbeck, C. (2015). Probabilistic Programming in Python using PyMC. *arXiv preprint arXiv:1507.08050*.