Probabilistic programming with Edward

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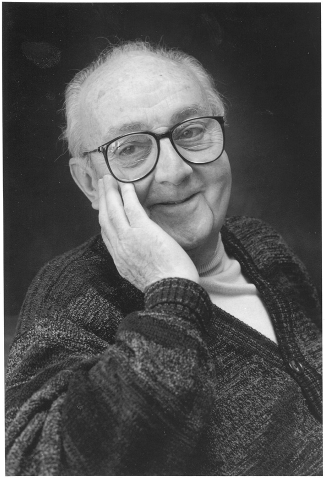
George E.P. Box (1919 - 2013)

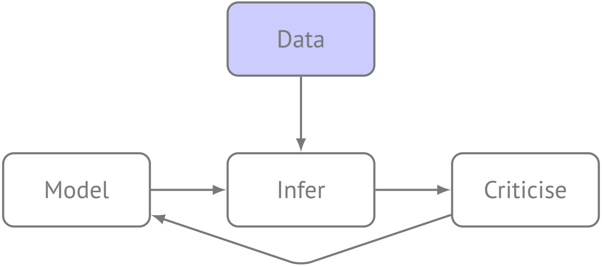


An iterative process for science:

1. Build a model of the science
2. Infer the model given data
3. Criticize the model given data

(Box and Hunter, 1962, 1965; Box and Hill, 1967; Box, 1976, 1980)

Box's Loop



Edward is a library designed around this loop
(Box, 1976, 1980; David M. Blei, 2014)

Edward is a probabilistic programming language, designed for fast experimentation and research (Tran et al., 2017).

Modelling

- Composable Turing-complete language of random variables
- Examples: Graphical models, neural networks, probabilistic programs
- Many data types, tensor vectorization, broadcasting, 3rd party support

Inference

- Composable language for hybrids, message passing, data subsampling
- Examples: Black box VI, Hamiltonian MC, stochastic gradient MCMC, generative adversarial networks
- Infrastructure to develop your own algorithms

Criticism

- Examples: Scoring rules, hypothesis tests, predictive checks

Built on TensorFlow (features distributed computing, GPUs, autodiff)

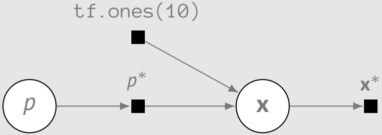
```python
# DATA
x_data = np.array([0, 1, 0, 0, 0, 0, 0, 0, 0, 1])

# MODEL
p = Beta(a=1.0, b=1.0)
x = Bernoulli(p=tf.ones(10) * p)

# VARIATIONAL DISTRIBUTION
qp_a = tf.nn.softplus(tf.Variable(tf.random_normal([])))
qp_b = tf.nn.softplus(tf.Variable(tf.random_normal([])))
qp = Beta(a=qp_a, b=qp_b)

# INFERENCE
inference = ed.KLqp({p: qp}, data={x: x_data})
inference.run(n_iter=500)

# CRITICISM
x_post = ed.copy(x, {p : qp})
def T(xs, zs):
  return tf.reduce_mean(xs[x_post])
ed.ppc(T, data={x_post: x_data})
```

Model code

```
p = Beta(a=1.0, b=1.0)
x = Bernoulli(p=tf.ones(10) * p)
```

The random variables p and x are represented by tensors p^* and $\mathbf{x}^*$ in the tensorflow computational graph

Computational graph



Random variables are equipped with methods for likelihoods $\log(x|p)$, expectations $\mathbb{E}_{p(x|p)}[x]$, and sampling $\sim p(x|p)$.

Graph can be executed by `x.value()` which returns the tensor $\mathbf{x}^*$ and simulates the generative process.

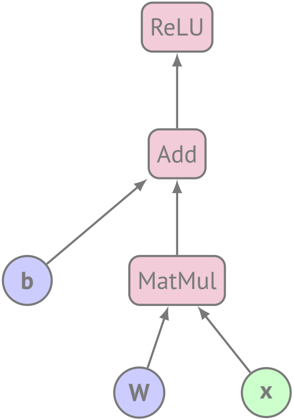
Tensorflow

$$h_i = \text{ReLU}(\mathbf{Wx} + \mathbf{b})$$

x is a placeholder for data

W, **b** are variables to store parameters across graph evaluations

MatMul, Add, and ReLU are operations



Model construction

Key concept is compositionality:

- Computational graphs can contain arbitrary tensorflow constructs
- Tensorflow conditional evaluations permit nonparametric processes
- Interface with third party tensorflow libraries, e.g. Keras for deep learning

Generative model

```
from edward.models import Bernoulli, Normal
from keras.layers import Dense

z = Normal(mu=tf.zeros([N, d]), sigma=tf.ones([N, d]))
h = Dense(256, activation='relu')(z.value())
x = Bernoulli(logits=Dense(28 * 28)(h))
```

Inference abstraction

Edward's random variables can represent probabilistic models as computational graphs.

How to perform inference? We desire:

- Support for many inference classes
- The posterior can be further composed as part of a larger model

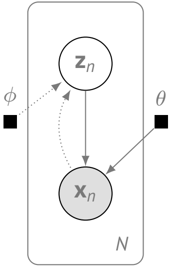
Edward abstracts this as an optimisation problem

$$\min_{\boldsymbol{\lambda},\boldsymbol{\theta}} \mathcal{L}(p(\mathbf{z} \mid \mathbf{x}; \theta), q(\mathbf{z}; \phi))$$

where q can be a variational distribution, point estimate or collection of samples.

The loss for the optimisation problem is encoded in the same computational graph as the model.

MNIST variational auto-encoder




```python
# Probabilistic model
z = Normal(mu=tf.zeros([N, d]), sigma=tf.ones([N, d]))
h = Dense(256, activation='relu')(z)
x = Bernoulli(logits=Dense(28 * 28, activation=None)(h))

# Variational model
qx = tf.placeholder(tf.float32, [N, 28 * 28])
qh = Dense(256, activation='relu')(qx)
qz = Normal(mu=Dense(d, activation=None)(qh),
            sigma=Dense(d, activation='softplus')(qh))
```

Inference

```python
inference = ed.KLqp({z: qz}, data={x: qx})
inference.initialize()

for epoch in range(n_epoch):
  for t in range(n_iter_per_epoch):
    inference.update(feed_dict={qx: mnist.train.next_batch(M)})
```

Criticism

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# MODEL
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# INFERENCE
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inference.run(n_iter=500)

# CRITICISM
x_post = ed.copy(x, {p : qp})
def T(xs, zs):
  return tf.reduce_mean(xs[x_post])
ed.ppc(T, data={x_post: x_data})
```

`ed.copy()`: conditioning as graph manipulation

Model comparisons

Inference method	Negative log-likelihood
VAE (Kingma & Welling, 2014)	≤ 88.2
VAE without analytic KL	≤ 89.4
VAE with analytic entropy	≤ 88.1
VAE with score function gradient	≤ 87.9
Normalizing flows (Rezende & Mohamed, 2015)	≤ 85.8
Hierarchical variational model (Ranganath et al., 2016b)	≤ 85.4
Importance-weighted auto-encoders ($K = 50$) (Burda et al., 2016)	≤ 86.3
HVM with IWAE objective ($K = 5$)	≤ 85.2
Rényi divergence ($\alpha = -1$) (Li & Turner, 2016)	≤ 140.5

Table 1: Inference methods for a probabilistic decoder on binarized MNIST. The Edward PPL makes it easy to experiment with many algorithms.

Semi-supervised learning

Model M2 from Kingma et al., 2014

$$y \sim \mathrm{Cat}(y|\pi)$$
$$\mathbf{z} \sim \mathcal{N}(0, I)$$
$$\mathbf{x}|y, \mathbf{z} \sim f(\mathbf{x}; y, \mathbf{z}, \theta)$$

55,000 binarized images, $\mathbf{x}$
3,000 have associated labels, y
f is a deconvolutional network
with a Bernoulli likelihood

Variational distribution

$$q_\phi(y|\mathbf{x}) = \mathrm{Cat}(\boldsymbol{\pi}_\phi(\mathbf{x}))$$
$$q_\phi(\mathbf{z}|y, \mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}_\phi(y, \mathbf{x}), \mathrm{diag}(\boldsymbol{\sigma}^2_\phi(\mathbf{x})))$$

Semi-supervised learning

Loss for labelled samples

$$\mathcal{L}(\mathbf{x}, y) = -\mathbb{E}_{q_\phi(\mathbf{z}|y,\mathbf{x})}[\log p_\theta(\mathbf{x}|y,\mathbf{z}) + \log p_\theta(y) + \log p(\mathbf{z}) - \log q_\phi(\mathbf{z}|y,\mathbf{x})]$$

Loss for unlabelled samples

$$\mathcal{U}(\mathbf{x}, y) = \sum_y q_\phi(y|\mathbf{x})\mathcal{L}(\mathbf{x}, y) - \mathcal{H}(q_\phi(y|x))$$

Gradients of KL-divergence and entropy are analytic

Reparameterisation trick

$$\nabla_{\{\theta,\phi\}}\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z})] = \mathbb{E}_{\mathcal{N}(\epsilon|\mathbf{0},\mathbf{I})}[\nabla_{\{\theta,\phi\}} \log p_\theta(\mathbf{x}|\boldsymbol{\mu}_\phi(\mathbf{x}) + \boldsymbol{\sigma}_\phi(\mathbf{x}) \odot \epsilon)]$$

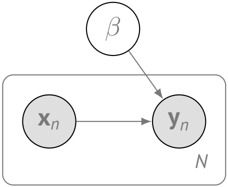
Semi-supervised learning

x sampled from generative model

y fixed in each row

z varies across columns

GPU-accelerated Hamiltonian Monte Carlo




```
# MODEL
x = tf.placeholder(tf.float32, [N, D])
beta = Normal(mu=tf.zeros(D), sigma=tf.ones(D))
y = Bernoulli(logits=ed.dot(x, beta))

# INFERENCE
qbeta = Empirical(params=tf.Variable(tf.random_normal([T, D])))
inference = ed.HMC({beta: qbeta}, data={y: y_data})
```

Bayesian logistic regression for the Covertype dataset ($N = 581012, D = 54$)
12-core Intel i7-5930K CPU at 3.50GHz and a NVIDIA Titan X (Maxwell) GPU
100 iterations of HMC

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

(Carpenter et al., 2017; Salvatier, Wiecki, and Fonnesbeck, 2015)

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[3] G. E. P. Box and W. J. Hill. “Discrimination among Mechanistic Models”. In: *Technometrics* 9.1 (1967), pp. 57–71. JSTOR: 1266318.

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