Probabilistic programming with Edward

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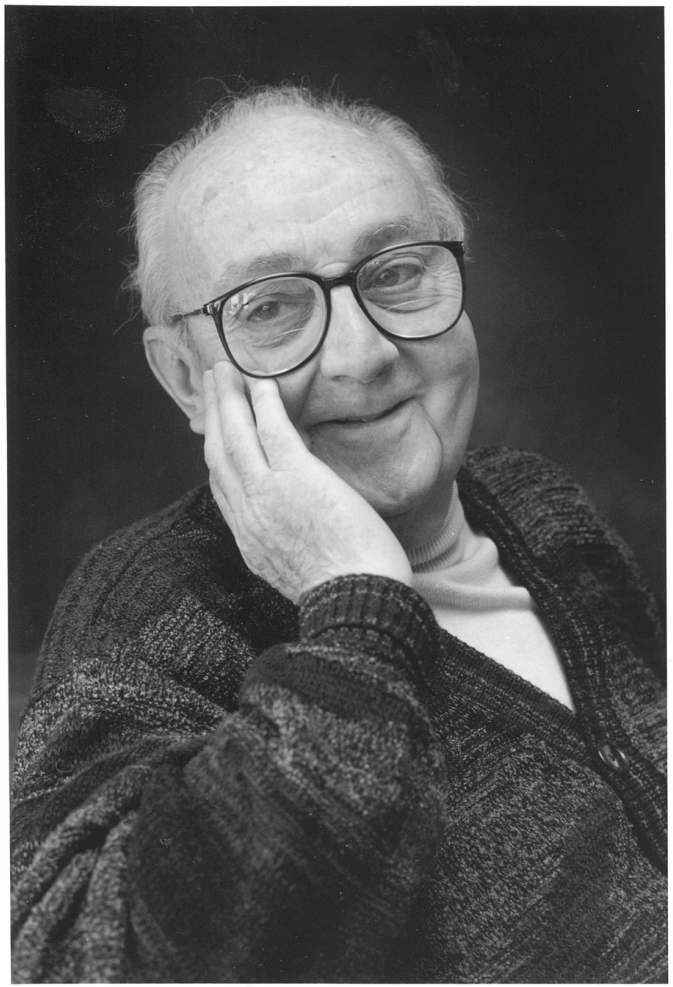
George E.P. Box (1919 - 2013)

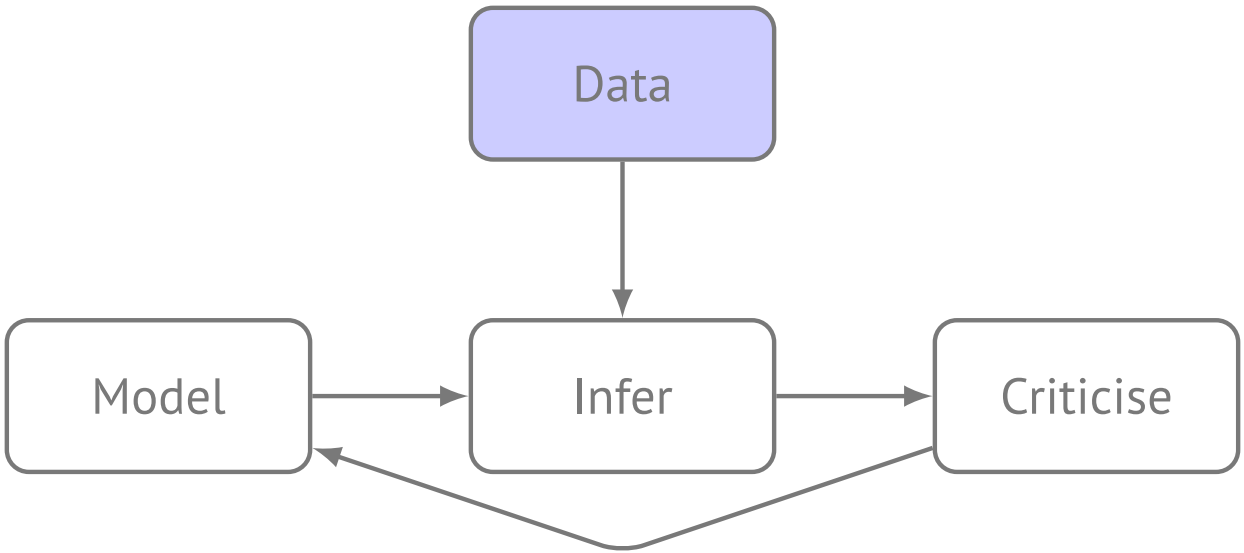


An iterative process for science:

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)

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.

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).

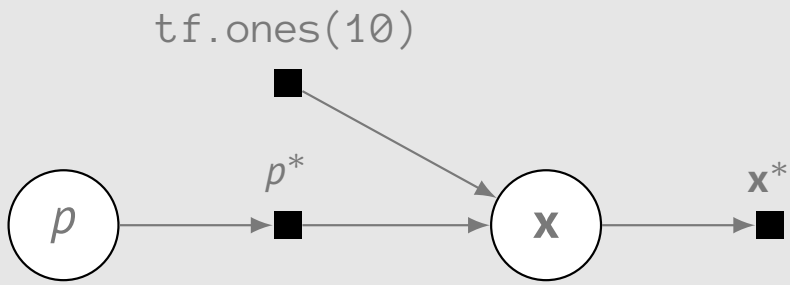
```
# DATA
x_data = np.array([0, 1, 0, 0, 0, 0, 0, 0, 0, 1])

# 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 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 x^* and simulates the generative process.

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

Deep 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

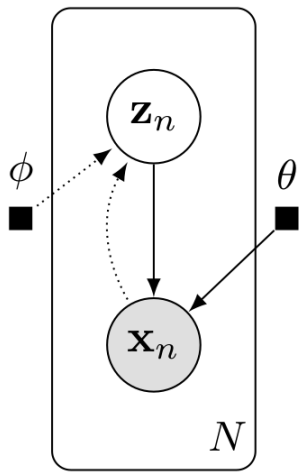
Edward abstracts this as an optimisation problem

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

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.

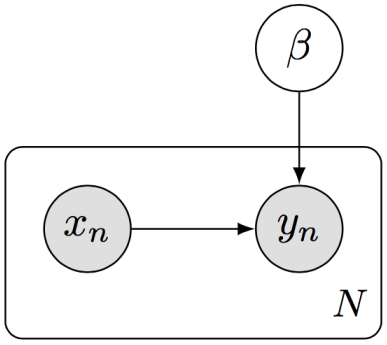
MNIST variational auto-encoder




```
1   # Probabilistic model
2   z = Normal(mu=tf.zeros([N, d]), sigma=tf.ones([N, d]))
3   h = slim.fully_connected(z, 256, activation_fn=tf.nn.relu)
4   x = Bernoulli(logits=slim.fully_connected(h, 28 * 28, activation_fn=None))
5
6   # Variational model
7   qx = tf.placeholder(tf.float32, [N, 28 * 28])
8   qh = slim.fully_connected(qx, 256, activation_fn=tf.nn.relu)
9   qz = Normal(mu=slim.fully_connected(qh, d, activation_fn=None),
10              sigma=slim.fully_connected(qh, d, activation_fn=tf.nn.softplus))
```

Figure 2: Variational auto-encoder for a data set of 28×28 pixel images: (left) graphical model, with dotted lines for the inference model; (right) probabilistic program, with 2-layer neural networks.

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)
```

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)

Semi-supervised learning

Model M2 from Kingma et al., 2014

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

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

Semi-supervised learning

posterior samples

[1] G. E. P. Box and William G. Hunter. “A Useful Method for Model-Building”. In: *Technometrics* 4.3 (1962), pp. 301–318. JSTOR: 1266570.

[2] G. E. P. Box and William G. Hunter. “The Experimental Study of Physical Mechanisms”. In: *Technometrics* 7.1 (1965), pp. 23–42. JSTOR: 1266125.

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

[4] George E. P. Box. “Science and Statistics”. In: *Journal of the American Statistical Association* 71.356 (1976), pp. 791–799. JSTOR: 2286841.

[5] George E. P. Box. “Sampling and Bayes’ Inference in Scientific Modelling and Robustness”. In: *Journal of the Royal Statistical Society. Series A (General)* 143.4 (1980), pp. 383–430. JSTOR: 2982063.

[6] David M. Blei. “Build, Compute, Critique, Repeat: Data Analysis with Latent Variable Models”. In: *Annual Review of Statistics and Its Application* 1.1 (2014), pp. 203–232.

[7] Dustin Tran et al. “Deep Probabilistic Programming”. In: (Jan. 13, 2017). arXiv: 1701.03757 [cs, stat].

[8] Bob Carpenter et al. “Stan : A Probabilistic Programming Language”. In: *Journal of Statistical Software* 76.1 (2017).

[9] John Salvatier, Thomas Wiecki, and Christopher Fonnesbeck. “Probabilistic Programming in Python Using PyMC”. In: (July 29, 2015). arXiv: 1507.08050 [stat].

[10] Diederik P. Kingma et al. “Semi-Supervised Learning with Deep Generative Models”. In: *Advances in Neural Information Processing Systems*. 2014, pp. 3581–3589.