Bayesian Layers

A Module for Neural Network Uncertainty

Code:
github.com/google/edward2

Dustin Tran[1] Michael W. Dusenberry[1] Mark van der Wilk[2] Danijar Hafner[1]

dustinvtran

[1] Google Brain [2] PROWLER.io

Summary

Coding up uncertainty models at CIFAR+ scale leads to bad times.

How do you build a Bayesian ResNet? Uncertainty for model-based RL? Support GPU/TPU and flexible training?

Core contributions:

- No reinventing the wheel. No new language. No new abstractions.
- Extend neural network library semantics to **distributions over functions**.
- Everything composes!

What goes into a neural network library?

```
__init__(
    units,
    activation=None,
    use_bias=True,
    kernel_initializer='glorot_uniform',
    bias_initializer='zeros',
    kernel_regularizer=None,
    bias_regularizer=None,
    activity_regularizer=None,
    kernel_constraint=None,
    bias_constraint=None,
    **kwargs
)
```

In all libraries, **layers** are the core building block.

Optimizers, losses, metrics, and GPU/TPU strategies are designed around them.

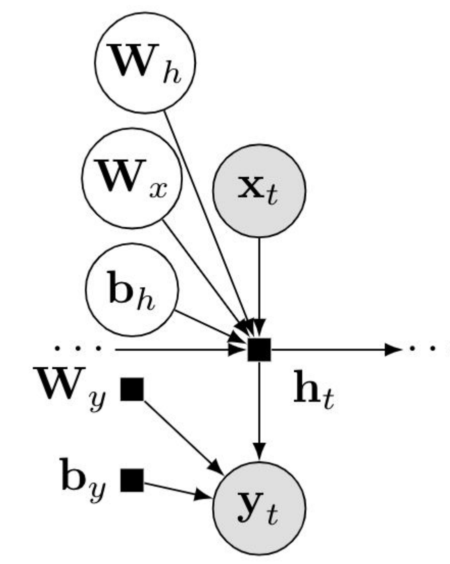
Initializers.
Regularizers.
Compositionality.

Example: Deep Gaussian Process

```
model = tf.keras.Sequential([
  tf.keras.layers.Flatten(),
  ed.layers.SparseGaussianProcess(units=256, num_inducing=512),
  ed.layers.SparseGaussianProcess(units=256, num_inducing=512),
  ed.layers.SparseGaussianProcess(units=10, num_inducing=512),
])

def loss_fn(features, labels):
  predictions = model(features)
  nll = tf.reduce_mean((labels-predictions.mean())**2)
  kl = sum(model.losses)
  return nll + kl/dataset_size

model.compile('adam', loss_fn)
model.fit(features, labels, batch_size=64, epochs=100)
```

Example: Bayesian LSTM

```
lstm = ed.layers.LSTMCellReparameterization(512)
output_layer = tf.keras.layers.Dense(10)

def loss_fn(features, labels, dataset_size):
  state = lstm.get_initial_state(features)
  nll = 0.
  for t in range(features.shape[1]):
    net, state = lstm(features[:, t], state)
    logits = output_layer(net)
    nll += tf.reduce_mean(
      tf.nn.softmax_cross_entropy_with_logits(
        labels[:, t], logits))

  kl = sum(lstm.losses) / dataset_size
  return nll + kl
```



Bayesian Layers

There are several design considerations for uncertainty models.

Computing the integral. We need to compute often-intractable integrals. For example in Bayesian neural networks:

$$\mathrm{ELBO}(\theta) = \int q(\theta) \log p(\mathbf{y} \mid f_\theta(\mathbf{x}))\, \mathrm{d}\theta - \mathrm{KL}\left[q(\theta) \,\|\, p(\theta)\right],$$

$$q(\mathbf{y} \mid \mathbf{x}) = \int q(\theta) p(\mathbf{y} \mid f_\theta(\mathbf{x}))\, \mathrm{d}\theta.$$

Make each estimator its own **Layer**.

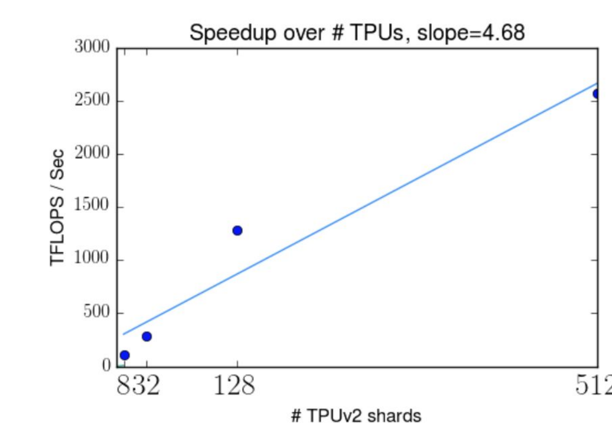
Type Signature. Bayesian layers are **drop-in replacements**.

```
if FLAGS.be_bayesian:
  Conv2D = layers.Conv2DReparameterization
else:
  Conv2D = tf.keras.layers.Conv2D

model = tf.keras.Sequential([
    Conv2D(32, kernel_size=5, strides=1, padding="SAME"),
    tf.keras.layers.BatchNormalization(),
    tf.keras.layers.Activation("relu"),
    Conv2D(32, kernel_size=5, strides=2, padding="SAME"),
    tf.keras.layers.BatchNormalization(),
    ...
])
```

Initializers. Extend to enable learnable distributions.
Regularizers. Extend to enable distributional penalties.

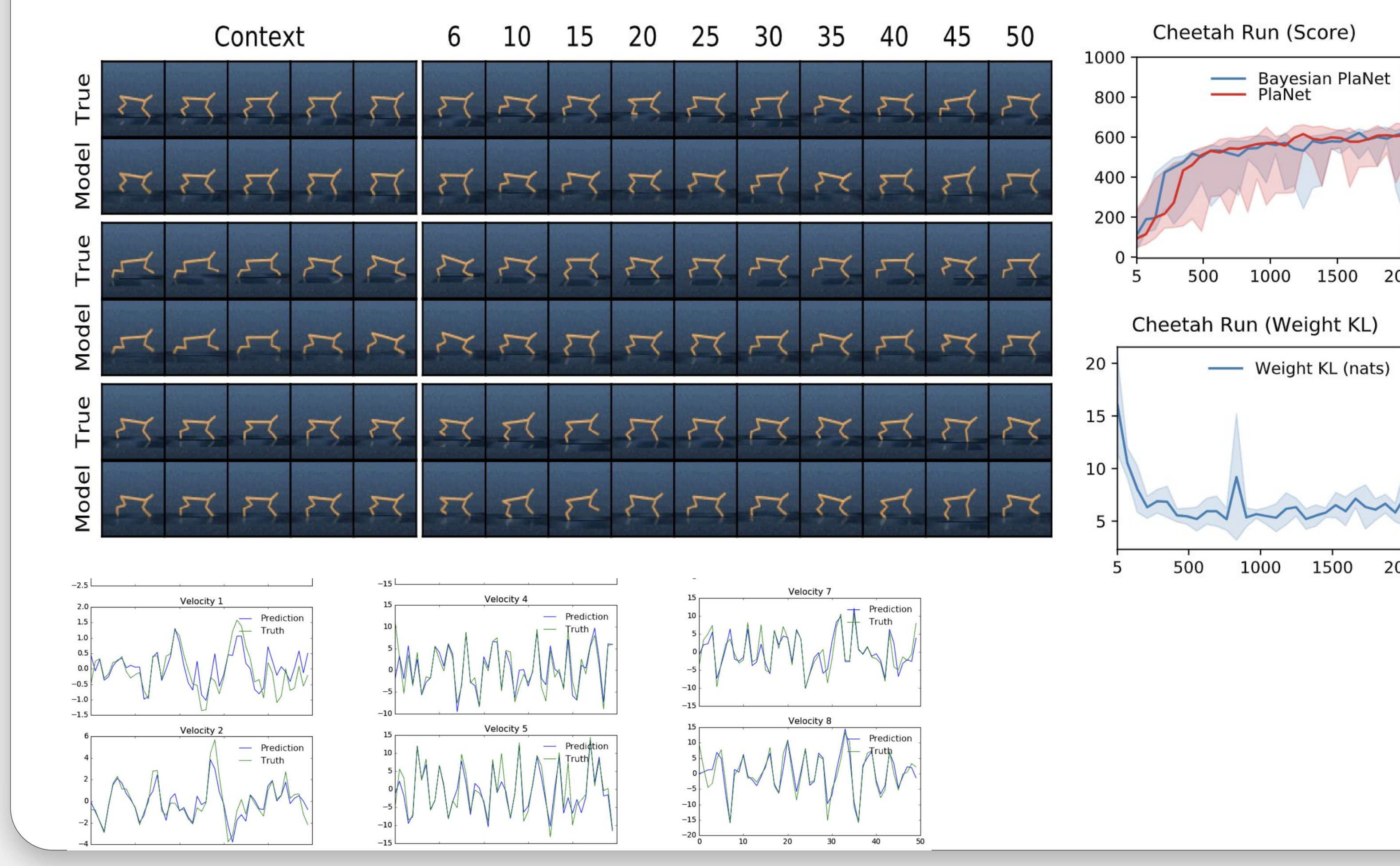
Experiments

Transformer (WMT EN-DE). Bayesian Layers lets us scale up seq2seq uncertainty models to 5 billion parameters over TPUs.



	BLEU	Calibration Error
Baseline	43.9	90.3%
Variational	43.8	20.8%

Planet (Half-Cheetah). Bayesian Layers integrates easily into existing workflows (here, TF Agents for model-based RL).



Current Work

Uncertainty baselines. High-quality, SOTA implementations of uncertainty models. (**note:** We already have CIFAR & ImageNet SOTA!)

- How does model uncertainty correlate with generalization?
- How do we combine SGD randomization with explicit prior/posterior randomization?
- How can uncertainty models achieve not just better robustness and reliability but better test accuracy?

Code: github.com/google/edward2