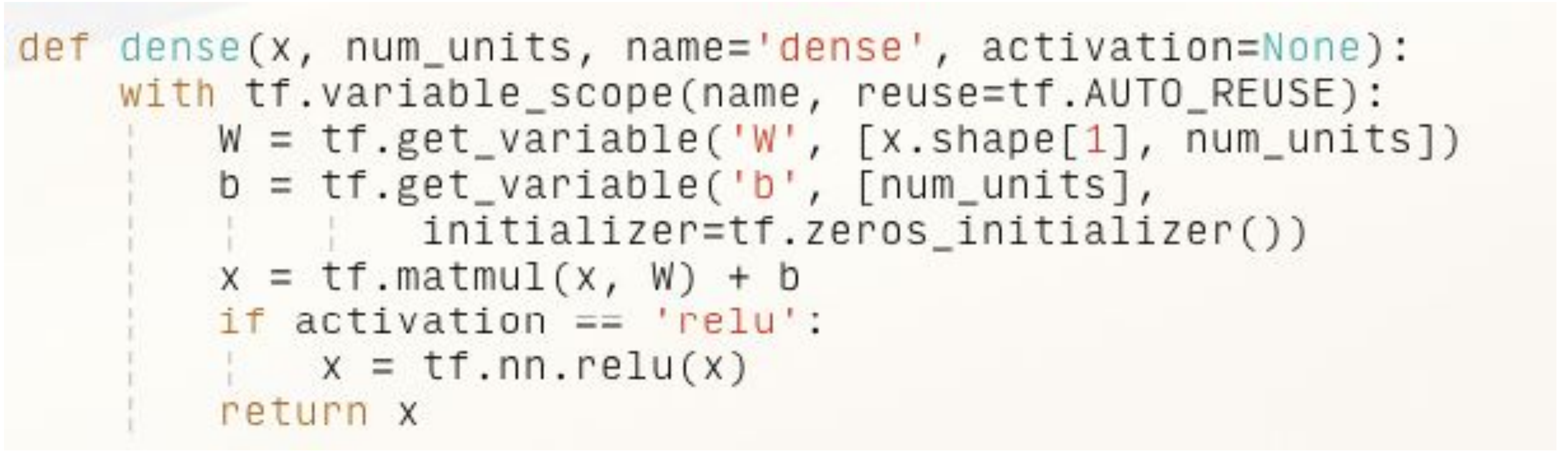
Implementing Bayes by Backprop

Juho Lee
Grad school of AI
Samsung AI expert course

`dense` layer in `tensorflow`



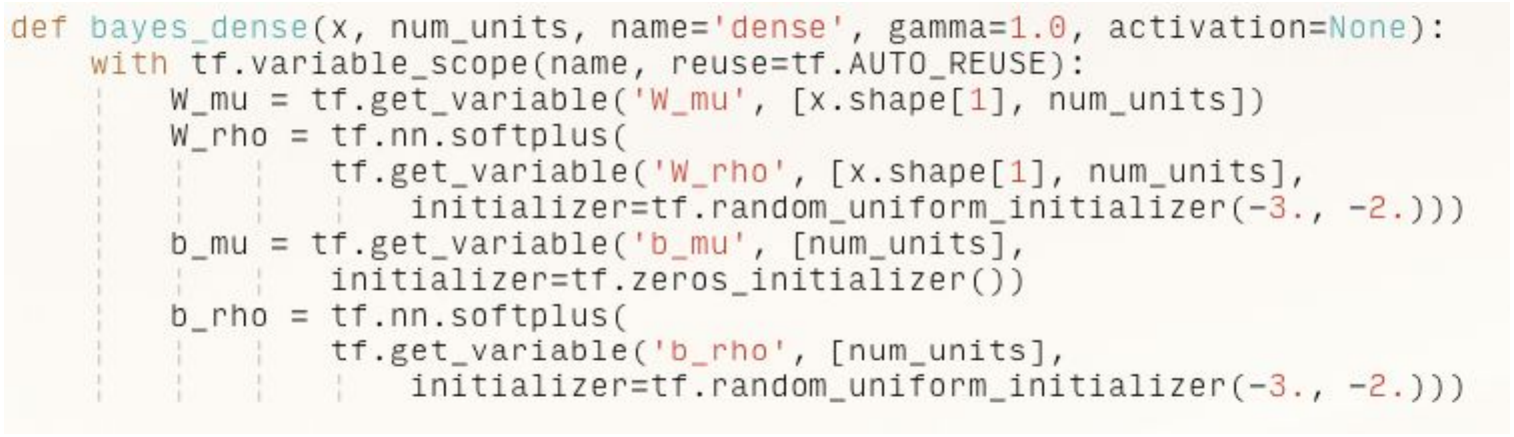
```python
def dense(x, num_units, name='dense', activation=None):
    with tf.variable_scope(name, reuse=tf.AUTO_REUSE):
        W = tf.get_variable('W', [x.shape[1], num_units])
        b = tf.get_variable('b', [num_units],
                initializer=tf.zeros_initializer())
        x = tf.matmul(x, W) + b
        if activation == 'relu':
            x = tf.nn.relu(x)
        return x
```

$$\mathbf{y} = \underbrace{\mathbf{x}}_{\boxed{\mathbb{R}^{N\times d_{\text{in}}}}}\underbrace{\mathbf{W}}_{\boxed{\mathbb{R}^{d_{\text{in}}\times d_{\text{out}}}}} + \underbrace{\mathbf{b}}_{\boxed{\mathbb{R}^{d_{\text{out}}}}}$$

Bayes Dense?

- Keep the distribution of W and b
- The distributions? - Gaussians
- To define Gaussians, we need means and covariances.

`bayes_dense` layers in `tensorflow`

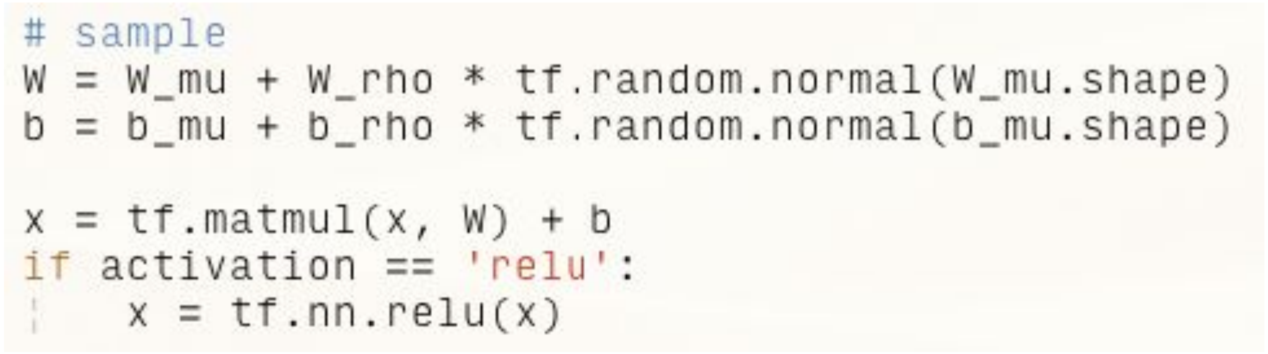


```python
def bayes_dense(x, num_units, name='dense', gamma=1.0, activation=None):
    with tf.variable_scope(name, reuse=tf.AUTO_REUSE):
        W_mu = tf.get_variable('W_mu', [x.shape[1], num_units])
        W_rho = tf.nn.softplus(
                tf.get_variable('W_rho', [x.shape[1], num_units],
                    initializer=tf.random_uniform_initializer(-3., -2.)))
        b_mu = tf.get_variable('b_mu', [num_units],
                initializer=tf.zeros_initializer())
        b_rho = tf.nn.softplus(
                tf.get_variable('b_rho', [num_units],
                    initializer=tf.random_uniform_initializer(-3., -2.)))
```

$$q(\mathbf{W}) = \mathcal{N}(\boldsymbol{\mu}_{\mathbf{W}}, \boldsymbol{\rho}^2_{\mathbf{W}}) = \prod_{i,j} \mathcal{N}(\mu_{w_{ij}}, \rho^2_{w_{ij}})$$

$$q(\mathbf{b}) = \mathcal{N}(\boldsymbol{\mu}_{\mathbf{b}}, \boldsymbol{\rho}^2_{\mathbf{b}}) = \prod_{j} \mathcal{N}(\mu_{b_j}, \rho^2_{b_j})$$

Computing outputs in `bayes_dense`



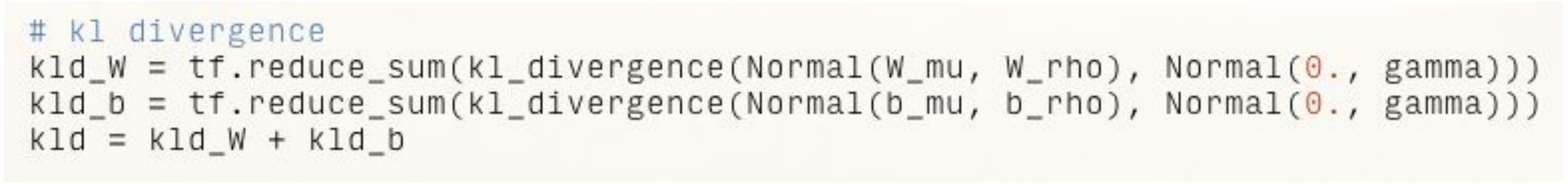
```
# sample
W = W_mu + W_rho * tf.random.normal(W_mu.shape)
b = b_mu + b_rho * tf.random.normal(b_mu.shape)

x = tf.matmul(x, W) + b
if activation == 'relu':
    x = tf.nn.relu(x)
```

$$\mathbf{W} = \boldsymbol{\mu}_{\mathbf{W}} + \boldsymbol{\varepsilon} \odot \boldsymbol{\rho}_{\mathbf{W}}, \quad \boldsymbol{\varepsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

$$\mathbf{b} = \boldsymbol{\mu}_{\mathbf{b}} + \boldsymbol{\varepsilon} \odot \boldsymbol{\rho}_{\mathbf{b}}, \quad \boldsymbol{\varepsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

KL-divergence



```
# kl divergence
kld_W = tf.reduce_sum(kl_divergence(Normal(W_mu, W_rho), Normal(0., gamma)))
kld_b = tf.reduce_sum(kl_divergence(Normal(b_mu, b_rho), Normal(0., gamma)))
kld = kld_W + kld_b
```

$$p(\mathbf{W}) = \mathcal{N}(\mathbf{0}, \gamma\mathbf{I}) \qquad p(\mathbf{b}) = \mathcal{N}(\mathbf{0}, \gamma\mathbf{I})$$

$$\begin{aligned}\mathrm{KL}[q(\mathbf{W})q(\mathbf{b})\|p(\mathbf{W})p(\mathbf{b})] =& \\ &\mathrm{KL}[q(\mathbf{W}\|p(\mathbf{W}] + \mathrm{KL}[q(\mathbf{b})\|p(\mathbf{b})]\end{aligned}$$