## TopogrElow

TensorFlow API r1.4

tf.contrib.bayesflow.hmc.leapfrog\_integrator

```
leapfrog_integrator(
    step_size,
    n_steps,
    initial_position,
    initial_momentum,
    potential_and_grad,
    initial_grad,
    name=None
)
```

Defined in tensorflow/contrib/bayesflow/python/ops/hmc\_impl.py.

Applies n\_steps steps of the leapfrog integrator.

This just wraps leapfrog\_step() in a tf.while\_loop(), reusing gradient computations where possible.

## Args:

- step\_size: Scalar step size or array of step sizes for the leapfrog integrator. Broadcasts to the shape of
  initial\_position. Larger step sizes lead to faster progress, but too-large step sizes lead to larger discretization
  error and worse energy conservation.
- n\_steps: Number of steps to run the leapfrog integrator.
- initial\_position: Tensor containing the value(s) of the position variable(s) to update.
- initial\_momentum: Tensor containing the value(s) of the momentum variable(s) to update.
- potential\_and\_grad: Python callable that takes a position tensor like **initial\_position** and returns the potential energy and its gradient at that position.
- initial\_grad: Tensor with the value of the gradient of the potential energy at initial\_position.
- name: Python str name prefixed to Ops created by this function.

## Returns:

- updated\_position: Updated value of the position.
- updated\_momentum: Updated value of the momentum.
- new\_potential: Potential energy of the new position. Has shape matching
   potential\_and\_grad(initial\_position).
- new\_grad: Gradient from potential\_and\_grad() evaluated at the new position. Has shape matching initial\_position.

Example: Simple quadratic potential.

```
def potential_and_grad(position):
  return tf.reduce_sum(0.5 * tf.square(position)), position
position = tf.placeholder(np.float32)
momentum = tf.placeholder(np.float32)
potential, grad = potential_and_grad(position)
new_position, new_momentum, new_potential, new_grad = hmc.leapfrog_integrator(
  0.1, 3, position, momentum, potential_and_grad, grad)
sess = tf.Session()
position_val = np.random.randn(10)
momentum_val = np.random.randn(10)
potential_val, grad_val = sess.run([potential, grad],
                                   {position: position_val})
positions = np.zeros([100, 10])
for i in xrange(100):
  position_val, momentum_val, potential_val, grad_val = sess.run(
    [new_position, new_momentum, new_potential, new_grad],
    {position: position_val, momentum: momentum_val})
  positions[i] = position_val
# Should trace out sinusoidal dynamics.
plt.plot(positions[:, 0])
```

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