

Efficiency of Univariate Kernel Density Estimation with TensorFlow

Bachelor Thesis

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Abstract

This study aims at comparing the speed and accuracy of differentu methods for one-dimensional kernel density estimation in Python/TensorFlow, especially concerning applications in high energy physics.

Starting from the basic algorithm, several optimizations from recent papers are introduced and combined to ameliorate the efficiency of the algorithm.

0.1 Kernel Density Estimation

Kernel Density Estimation[@rosenblatt1956] has improved, see figure [@fig:kde].

```
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
import tensorflow as tf
import tensorflow_probability as tfp
from zfit_benchmark.timer import Timer
import zfit as z
```

1 Methods

1.1 Generation of Test Distribution

Listing: Test Distribution generation

```
r_{seed} = 1978239485
n_datapoints = 1000000
tfd = tfp.distributions
mix_3gauss_1exp_1uni = tfd.Mixture(
  cat=tfd.Categorical(probs=[0.1, 0.2, 0.1, 0.4, 0.2]),
  components=[
    tfd.Normal(loc=-1., scale=0.4),
    tfd.Normal(loc=+1., scale=0.5),
    tfd.Normal(loc=+1., scale=0.3),
    tfd.Exponential(rate=2),
    tfd.Uniform(low=-5, high=5)
])
data =
→ mix_3gauss_1exp_1uni.sample(sample_shape=n_datapoints,

    seed=r_seed).numpy()
```

```
ax = plt.gca()
n_{\text{testpoints}} = 200
fac1 = 1.0 / np.sqrt(2.0 * np.pi)
exp_fac1 = -1.0/2.0
h1 = 0.01
y_fac1 = 1.0/(h1*n_datapoints)
with Timer ("Benchmarking") as timer:
    with timer.child('tf.simple-kde'):
        @tf.function(autograph=False)
        def tf_kde():
            fac = tf.constant(fac1, tf.float64)
            exp_fac = tf.constant(exp_fac1, tf.float64)
            y_fac = tf.constant(y_fac1, tf.float64)
```

```
h = tf.constant(h1, tf.float64)
           data_tf = tf.convert_to_tensor(data, tf.float64)
           gauss_kernel = lambda x: tf.math.multiply(fac,

    tf.math.exp(tf.math.multiply(exp_fac,

    tf.math.square(x))))
           calc_value = lambda x: tf.math.multiply(y_fac,

    tf.math.reduce_sum(gauss_kernel(tf.math.divide(tf.math.subtract(x,

¬ data_tf), h))))
           x = tf.linspace(tf.cast(-5.0, tf.float64),

    tf.cast(5.0, tf.float64), num=tf.cast(n_testpoints,

  tf.int64))
           y = tf.zeros(n_testpoints)
           return x, tf.map_fn(calc_value, x)
       x, y = tf_kde()
       sns.lineplot(x, y, ax=ax)
       timer.stop()
  with timer.child('simple-kde'):
       fac = fac1
       exp_fac = exp_fac1
```

```
y_fac = y_fac1
     h = h1
     gauss_kernel = lambda x: fac * np.exp(exp_fac * x**2)
     x2 = np.linspace(-5.0, 5.0, num=n_testpoints)
     y2 = np.zeros(n_testpoints)
     for i, x_i in enumerate(x2):
        y2[i] = y_fac * np.sum(gauss_kernel((x_i-data)/h))
     sns.lineplot(x2,y2, ax=ax)
     timer.stop()
 with timer.child('sns.distplot'):
     plot = sns.distplot(data, bins=1000, kde=True,
rug=False, ax=ax)
     timer.stop()
```

<matplotlib.axes._subplots.AxesSubplot object at 0x7fa57661db50>
<matplotlib.axes._subplots.AxesSubplot object at 0x7fa57661db50>

```
print(timer.child('tf.simple-kde').elapsed)
```

1.4875598099999999929263943457

```
print(timer.child('simple-kde').elapsed)
```

1.600860774000000930072928895

```
print(timer.child('sns.distplot').elapsed)
```

1.196890326000001891770807561

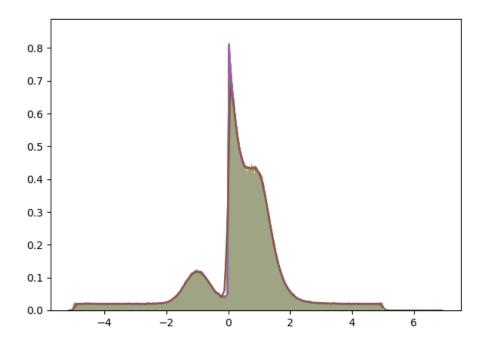


Figure 1: Kernel Density Estimation

$$\mathbf{r} \equiv egin{bmatrix} y \ heta \end{bmatrix}$$

{#eq:eq1}

2 Abstract

This study aims at comparing the speed and accuracy of differentu methods for one-dimensional kernel density estimation in Python/TensorFlow, especially concerning applications in high energy physics.

Starting from the basic algorithm, several optimizations from recent papers are introduced and combined to ameliorate the efficiency of the algorithm.

3 Literature

Here is a review of existing methods.

4 Methods

We describe our methods in this chapter.

5 Final Words

We have finished a nice book.

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Listings