

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.

1 Introduction

2 Literature

Here is a review of existing methods.¹

3 Methods

We describe our methods in this chapter.

```
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
```

3.1 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_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 0x7fa8d2341dd0>
## <matplotlib.axes._subplots.AxesSubplot object at 0x7fa8d2341dd0>
```

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

1.471278211999997864722899976

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

1.548966466999999624931660946

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

1.123539057999998647119355155

plt.savefig('plots/kde.png')

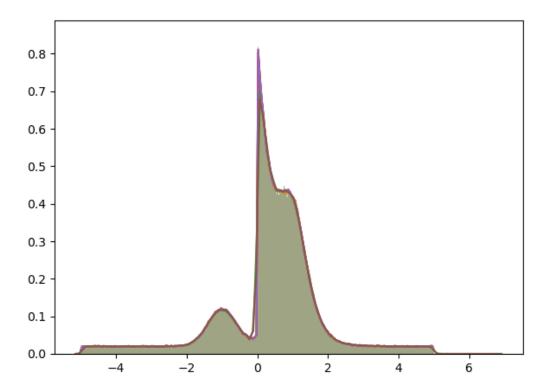


Figure 1: Kernel Density Estimation

$$\mathbf{r} \equiv \begin{bmatrix} y \\ \theta \end{bmatrix} \tag{1}$$

4 Final Words

We have finished a nice book.

References

¹ M. Rosenblatt, (1956).

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