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1  #!/usr/bin/python3
2
3  import random
4
5  import matplotlib.pyplot as plt
6  import numpy as np
7  import tensorflow as tf
8  import matplotlib.patches as mpatches
9
10 from matplotlib.colors import ListedColormap
11 from tqdm import trange
12
13 NUM_SAMPLES = 1000
14 INPUT_NOISE = 0.5
15
16 BATCH_SIZE = 1000
17 NUM_BATCHES = 3000
18 NUM_FEATURES = 2
19 BETA = 0.001
20
21 FIRST_LAYER = 1024
22 SECOND_LAYER = 32
23 THIRD_LAYER = 16
24 FOURTH_LAYER = 4
25 OUTPUT_LAYER = 1
26
27 NUM_LAYERS = 5
28
29 random.seed(42)
30
31 """
32 I have learned that the choice of initialization and activation functions drastically
33 changes the performance of overall function. For the initialization, I initially tried
34 with normal, but the model failed randomly with extreme case of normal initialization.
35 Secondly, I tried truncated_normal to avoid samples over and below two standard deviation,
36 to avoid the saturation region when I tried sigmoid or tanh activation functions.
37 And then, I researched about popular initialization methods and found out glorot_uniform
38 that is default initializer for keras models. Glorot_uniform depends on the the number
39 of input units in the weight tensor and the number of output units in the weight distribution
40 to find the limit of uniform distribution  $U(-limit, limit)$  where  $limit = \sqrt{6/(\#in + \#out)}$ .
41 With the Glorot_uniform, the model converged more stably.
42
43 For the activation functions, Sigmoid was not considered to be a part of f because of
44 the gradient vanishing. There are only 5 layers, so the gradient is at least reduced by
45  $(1/4)^5$  at the output. Tanh seemed to work fine but the output boundary line seemed to
46 be easily overfitting. Lastly, relu and its variations (elu, relu6, leaky_relu) were
47 considered to avoid the gradient vanishing, and there is not much of difference, but elu
48 seems to be the one that best generalize.
49
50 Also, the number of layers was started with 4 layers because spiral dataset is a non-linear
51 function that does not look similar to activation functions that we commonly use. Therefore,
52 multiple layers were considered initially. And, I read in one of the textbooks that latter
53 layers learn higher-level information compared to earlier layers, so I tried to increase the
54 number
55 of layer instead of increasing the size of each layer. And later on, I tried to increase the
56 size of
57 earlier layers and decrease the size of latter layer in an assumption that the higher-level
58 information
59 requires more lower-level information to have a firm foundation. The layer sizes were selected
60 with power
61 of two for optimization for matrix operations.
62 """
63
64 class Data(object):
65     def __init__(self):
66         # spiral generation code snippets inspiration
67         https://gist.github.com/ld86/497e2bcb917d828f3ccd6922345571bd
68         half_samples = NUM_SAMPLES // 2
69         theta = (1 + 1.75 * np.random.rand(NUM_SAMPLES)) * 2 * np.pi
70         x = (

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67         np.concatenate(
68             (
69                 -theta[:half_samples] * np.cos(theta[:half_samples]),
70                 theta[half_samples:] * np.cos(theta[half_samples:]),
71             )
72         )
73     + np.random.rand(NUM_SAMPLES) * INPUT_NOISE
74 )
75 y = (
76     np.concatenate(
77         (
78             -theta[:half_samples] * np.sin(theta[:half_samples]),
79             theta[half_samples:] * np.sin(theta[half_samples:]),
80         )
81     )
82     + np.random.rand(NUM_SAMPLES) * INPUT_NOISE
83 )
84
85 self.X = np.vstack((x, y)).T
86 self.X = self.X.astype("float32")
87 self.label = (
88     np.concatenate((np.zeros(half_samples), np.ones(half_samples)))
89     .astype("float32")
90     .reshape(NUM_SAMPLES, 1)
91 )
92 self.idx = np.arange(NUM_SAMPLES)
93
94 def get_batch(self, batch_size=BATCH_SIZE):
95     choices = np.random.choice(self.idx, size=batch_size)
96     return self.X[choices, :], self.label[choices]
97
98
99 class Model(tf.Module):
100     def __init__(self):
101         self.initializer = tf.initializers.GlorotUniform()
102
103         w1, b1 = self.generate_layer(NUM_FEATURES, FIRST_LAYER, "w1", "b1", False)
104         w2, b2 = self.generate_layer(FIRST_LAYER, SECOND_LAYER, "w2", "b2", False)
105         w3, b3 = self.generate_layer(SECOND_LAYER, THIRD_LAYER, "w3", "b3", False)
106         w4, b4 = self.generate_layer(THIRD_LAYER, FOURTH_LAYER, "w4", "b4", False)
107         w5, b5 = self.generate_layer(FOURTH_LAYER, OUTPUT_LAYER, "w5", "b5", True)
108
109         self.weights = [w1, w2, w3, w4, w5]
110         self.biases = [b1, b2, b3, b4, b5]
111
112     def generate_layer(
113         self, input_layer_size, out_layer_size, weight_name, bias_name, out
114     ):
115         w = tf.Variable(
116             self.initializer(shape=(input_layer_size, out_layer_size)), name=weight_name
117         )
118         if out:
119             b = tf.Variable(tf.zeros(shape=(1, 1)), name=bias_name)
120         else:
121             b = tf.Variable(tf.zeros(shape=(1, out_layer_size)), name=bias_name)
122         return w, b
123
124     def __call__(self, x):
125         for idx, (w, b) in enumerate(zip(self.weights, self.biases)):
126             x = x @ w + b
127             if idx + 1 == NUM_LAYERS:
128                 x = tf.math.sigmoid(x)
129             else:
130                 x = tf.nn.relu(x)
131         return x
132
133
134 if __name__ == "__main__":
135     data = Data()
136     model = Model()
137
138     optimizer = tf.optimizers.Adam()

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139
140 bar = trange(NUM_BATCHES)
141 for i in bar:
142     with tf.GradientTape() as tape:
143         X, y = data.get_batch()
144         y_hat = model(X)
145         loss = tf.reduce_mean(tf.losses.binary_crossentropy(y_true=y, y_pred=y_hat))
146         for w in model.weights:
147             loss += tf.nn.l2_loss(w) * BETA
148         grads = tape.gradient(loss, model.variables)
149         optimizer.apply_gradients(zip(grads, model.variables))
150         bar.set_description(f"Loss @ {i} => {loss.numpy():0.6f}")
151         bar.refresh()
152
153 plt.subplot(2, 1, 1)
154 plt.scatter(
155     data.X[:, 0],
156     data.X[:, 1],
157     c=np.squeeze(data.label),
158     cmap=ListedColormap(["#FF0000", "#0000FF"]),
159 )
160 class_zero = mpatches.Patch(color="#FF0000", label="class 0")
161 class_one = mpatches.Patch(color="#0000FF", label="class 1")
162
163 plt.title("ground truth")
164 plt.xlabel("x")
165 plt.ylabel("y").set_rotation(0)
166 plt.legend(handles=[class_zero, class_one])
167
168 plt.subplot(2, 1, 2)
169 plt.scatter(
170     data.X[:, 0],
171     data.X[:, 1],
172     c=np.squeeze(model(data.X) > 0.5),
173     cmap=ListedColormap(["#FF0000", "#0000FF"]),
174 )
175 class_zero = mpatches.Patch(color="#FF0000", label="class 0")
176 class_one = mpatches.Patch(color="#0000FF", label="class 1")
177
178 plt.title("predicted classes")
179 plt.xlabel("x")
180 plt.ylabel("y").set_rotation(0)
181 plt.legend(handles=[class_zero, class_one])
182
183 x, y = np.meshgrid(
184     np.linspace(np.min(data.X[:, 0]), np.max(data.X[:, 0]), 200),
185     np.linspace(np.min(data.X[:, 1]), np.max(data.X[:, 1]), 200),
186 )
187
188 z = np.vstack((x.flatten(), y.flatten())).T
189 z = tf.reshape(model(z), x.shape)
190
191 plt.contour(x, y, np.squeeze(z), levels=1, colors="k")
192
193 plt.show()
194

```