Mathematical Foundation of DNN : HW 6

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1

Let $D_p(\cdot)$ define as follows:

$$D_p(x) = \begin{cases} 0 \text{ with probability } p \\ x/(1-p) \text{ with probability } 1-p \end{cases} \tag{1}$$

For the case of ReLU and LeakyReLU, the dropout can be commutative. Let f denote the ReLU Leaky ReLU.

$$\begin{aligned} D_p(f(h)) &= \begin{cases} 0 \text{ with probability } p \\ f(h)/(1-p) \text{ with probability } 1-p \end{cases} && (\because \text{ the defition of dropout}) \\ &= \begin{cases} 0 \text{ with probability } p \\ f(h/(1-p)) \text{ with probability } 1-p \end{cases} && (\because f(ax) = af(x)\ \forall x, a > 0) \\ &= f(D_p(h)) \end{aligned}$$

However, for the sigmoid, we cannot do same thing to the discussion above since it is not homogeneous function. In addition, there is a trivial counter-example. Consider the hidden layer with element $[0, 0, 1]$. If we do dropout first, the last node can be zero with probability p and it results in $[0, 0, 0]$. Then, after applying the sigmoid function, the all three elements in the output must be same. However, if we do sigmoid activation first, since $Sigmoid(0) \neq 0$, the intermediate layer would be $[\sigma(0), \sigma(0), \sigma(1)]$. Although dropout cannot change their value to be evenly, they are not same to the result of Dropout-Sigmoid.

2

In this problem, I denote the bold symbol of each variable as the random variable corresponding to it.

$$\mathbb{E}[\mathbf{x}^{(i)}] = 0, \quad \mathbb{E}\left[\left(\mathbf{x}^{(i)}\right)^2\right] = 1$$

From the PyTorch offficial document, it is important to note the following relations.

$$\mathbf{A_l^{(ij)}} \sim \mathcal{U}\left(-\sqrt{\frac{3}{n_{l-1}}}, \sqrt{\frac{3}{n_{l-1}}}\right)$$
$$\mathbf{b_l^{(i)}} \sim \mathcal{U}\left(-\sqrt{\frac{1}{n_{l-1}}}, \sqrt{\frac{1}{n_{l-1}}}\right)$$

The relations above imply the following.

$$\mathbb{E}[\mathbf{A_l^{(ij)}}] = 0, \quad \mathbb{E}[\mathbf{b_l^{(i)}}] = 0$$
$$\mathbb{E}\left[\left(\mathbf{A_l^{(ij)}}\right)^2\right] = \frac{1}{n_{l-1}}, \quad \mathbb{E}\left[\left(\mathbf{b_l^{(i)}}\right)^2\right] = \frac{1}{3n_{l-1}}$$

Then, to derive the mean of $\mathbf{y}_L$, consider the mathematical induction of $\mathbb{E}[\mathbf{y}_l^{(i)}]$. For the base case, the mean value of $\mathbf{y}_1^{(i)}$ is zero.

$$\begin{aligned} \mathbb{E}[\mathbf{y_1^{(i)}}] &= \sum_{j=1}^{n_0} \mathbb{E}\left[\mathbf{A_l^{(ij)}}\mathbf{x^{(j)}}\right] + \mathbb{E}\left[\mathbf{b_1^{(i)}}\right] \\ &= \sum_{j=1}^{n_0} \mathbb{E}\left[\mathbf{A_l^{(ij)}}\right]\mathbb{E}\left[\mathbf{x^{(j)}}\right] \\ &= 0 \end{aligned}$$

Then, for the inductive step, the mean value of $\mathbf{y}_l^{(i)}$ is zero. To proof it, consider the following induction hypothesis: $\mathbb{E}[\mathbf{y}_{l-1}^{(i)}] = 0$.

$$\begin{aligned}
\mathbb{E}[\mathbf{y_l^{(i)}}] &= \sum_{j=1}^{n_{l-1}} \mathbb{E}\left[\mathbf{A_l^{(ij)}} \mathbf{y_{l-1}^{(j)}}\right] + \mathbb{E}\left[\mathbf{b_l^{(i)}}\right] \\
&= \sum_{j=1}^{n_{l-1}} \mathbb{E}\left[\mathbf{A_l^{(ij)}}\right] \mathbb{E}\left[\mathbf{y_{l-1}^{(j)}}\right] \\
&= 0
\end{aligned}$$

Next, I'll derive the variance of $\mathbf{y}_l^{(i)}$.

$$\begin{aligned}
\mathbb{E}\left[\left(\mathbf{y}_l^{(i)}\right)^2\right] &= \mathbb{E}\left[\left(\sum_j \mathbf{A}_l^{(ij)} \mathbf{y}_{l-1}^{(j)} + \mathbf{b}_l^{(i)}\right)^2\right] \\
&= \mathbb{E}\left[\sum_j \sum_k \mathbf{A}_l^{(ij)} \mathbf{A}_l^{(ik)} \mathbf{y}_{l-1}^{(j)} \mathbf{y}_{l-1}^{(k)} + 2\mathbf{b}_l^{(i)} \sum_j \mathbf{A}_l^{(ij)} \mathbf{y}_{l-1}^{(j)} + \left(\mathbf{b}_l^{(i)}\right)^2\right] \\
&= \mathbb{E}\left[\sum_j \sum_k \mathbf{A}_l^{(ij)} \mathbf{A}_l^{(ik)} \mathbf{y}_{l-1}^{(j)} \mathbf{y}_{l-1}^{(k)}\right] + \mathbb{E}\left[2\mathbf{b}_l^{(i)} \sum_j \mathbf{A}_l^{(ij)} \mathbf{y}_{l-1}^{(j)}\right] + \mathbb{E}\left[\left(\mathbf{b}_l^{(i)}\right)^2\right] \\
&= \sum_j \sum_k \mathbb{E}\left[\mathbf{A}_l^{(ij)} \mathbf{A}_l^{(ik)}\right] \mathbb{E}\left[\mathbf{y}_{l-1}^{(j)} \mathbf{y}_{l-1}^{(k)}\right] + \frac{1}{3n_{l-1}} \\
&= \sum_j \sum_k \frac{1}{n_{l-1}} \delta_{jk} \mathbb{E}\left[\mathbf{y}_{l-1}^{(j)} \mathbf{y}_{l-1}^{(k)}\right] + \frac{1}{3n_{l-1}} \\
&= \sum_j \frac{1}{n_{l-1}} \mathbb{E}\left[\left(\mathbf{y}_{l-1}^{(j)}\right)^2\right] + \frac{1}{3n_{l-1}}
\end{aligned}$$

As the result above says, $\mathbb{E}\left[\left(\mathbf{y}_l^{(i)}\right)^2\right]$ actually doesn't depend on the index i. This implies that $\mathbb{E}\left[\left(\mathbf{y}_l^{(1)}\right)^2\right] = \mathbb{E}\left[\left(\mathbf{y}_l^{(2)}\right)^2\right] = \cdots = \mathbb{E}\left[\left(\mathbf{y}_l^{(n_l)}\right)^2\right]$. From induction, this must be held on the $l-1$ layers.(Note that we can see the base case if we put $l = 1$ on the last equation above). Thus,

$$\begin{aligned}
\mathbb{E}\left[\left(\mathbf{y}_l^{(i)}\right)^2\right] &= \mathbb{E}\left[\left(\mathbf{y}_{l-1}^{(i)}\right)^2\right] + \frac{1}{3n_{l-1}} \\
\sum_{l=1}^{L} \mathbb{E}\left[\left(\mathbf{y}_l^{(i)}\right)^2\right] - \mathbb{E}\left[\left(\mathbf{y}_{l-1}^{(i)}\right)^2\right] &= \sum_{l=1}^{L} \frac{1}{3n_{l-1}} \\
\therefore \mathbb{E}\left[\left(\mathbf{y}_L^{(i)}\right)^2\right] &= 1 + \sum_{l=1}^{L} \frac{1}{3n_{l-1}}
\end{aligned}$$

3

I refer to the result of HW4-6 to solve this problem.

i

From the problem 6-(a) in HW4, we saw that $\frac{\partial}{\partial y_{l-1}} \sigma(A_l y_{l-1}) + b_l = \operatorname{diag}(\sigma'(A_l y_{l-1} + b_l))A_l$. Thus,

$$\begin{aligned}
y_l &= \sigma(A_l y_{l-1} + b_l) + y_{l-1} \\
\frac{\partial y_l}{\partial y_{l-1}} &= \operatorname{diag}\left(\sigma'(A_l y_{l-1} + b_l)\right) A_l + I_m
\end{aligned}$$

Here, I_m denotes the identity with dimension m.

ii

Since b_l and A_l are independent to y_{l-1}, we can directly use the result of problem 6 at HW4(with simple chain rule).

$$\frac{\partial y_L}{\partial b_l} = \frac{\partial y_L}{\partial y_l}\frac{\partial y_l}{\partial b_l} = \frac{\partial y_L}{\partial y_l}\text{diag}(\sigma'(A_l y_{l-1} + b_l))$$
$$\frac{\partial y_L}{\partial A_l} = \text{diag}(\sigma'(A_l y_{l-1}) + b_l)\left(\frac{\partial y_L}{\partial y_l}\right)^T y_{l-1}^T$$

iii

Both $\frac{\partial y_L}{\partial b_i}$ and $\frac{\partial y_L}{\partial A_i}$ contain $\frac{\partial y_L}{\partial y_i}$ term. According to the chain rule,

$$\frac{\partial y_L}{\partial y_i} = \frac{\partial y_L}{\partial y_{L-1}} \cdot \frac{\partial y_{L-1}}{\partial y_{L-2}} \cdots \frac{\partial y_{i+1}}{\partial y_i} = \prod_{k=i+1}^{L} \frac{\partial y_k}{\partial y_{k-1}} = \prod_{k=i+1}^{L} \text{diag}\left(\sigma'(A_k y_{k-1} + b_k)\right) A_k + I_m$$

As the equations above tell, eventhough $A_j = 0$ for some $j \in \{l+1, \cdots, L-1\}$ or $\sigma'(A_j y_{j-1} + b_j) = 0$ for some $j \in \{l+1, \cdots, L-1\}$, the identity matrices are still alive. Thus, the derivatives do not have to be zero. Note that the other components in both derivatives also are nonzero, in general.

4

a

In this problem, I used the following formula.

$$\text{trainable parameter} = (\text{kernel size})^2 \times C_{out} \times C_{in} + C_{out}$$

The overall calculation of the first convolution layer is as follow.

$$(128 \times 1^2 \times 256 + 128) + (128 \times 3^2 \times 128 + 128) + (256 \times 1^2 \times 128 + 256) = 213,504$$

For the second implementation, considering that each path have the same number of the trainable paramters, I calculated the number of trainable paramters for a single path. The whole calculation process is as follow.

$$(256 \times 1^2 \times 4 + 4) + (4 \times 3^2 \times 4 + 4) + (4 \times 1^2 \times 256 + 256) = 2456$$
$$\therefore 32 \times 2456 = 78,592$$

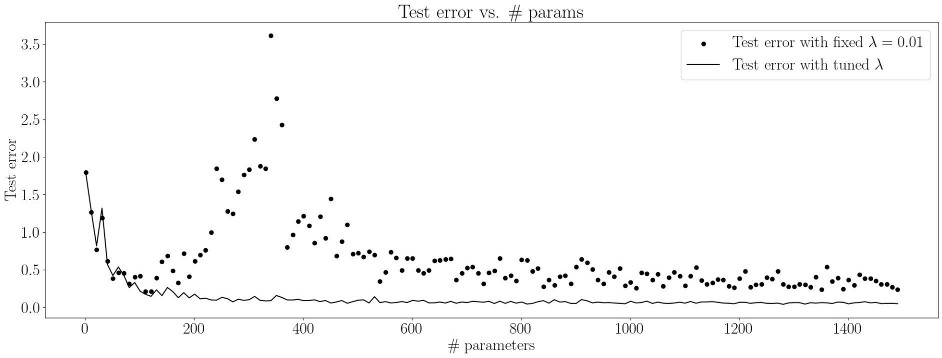
b

```
class STMConvLayer(nn.Module):
    def __init__(self):
        super(STMConvLayer, self).__init__()
        self.conv = nn.ModuleList()
        for _ in range(32):
            self.conv.append(
                nn.Sequential(
                    nn.Conv2d(256, 4, 1, dtype=torch.float),  # Specify dtype=torch.float
                    nn.ReLU(),
                    nn.Conv2d(4, 4, 3, padding=1, dtype=torch.float),  # Specify dtype=torch.
                                                                        float
                    nn.ReLU(),
                    nn.Conv2d(4, 256, 1, dtype=torch.float)  # Specify dtype=torch.float
                )
            )
    def forward(self,x): # x : bathced data
        output = torch.zeros(x.shape, dtype=torch.float)
        for path in self.conv:
            output += path(x.float())
        return output
```

The structure of my STMConvLayer is as follow. The followings are produced by print() function.

```
STMConvLayer(
  (conv): ModuleList(
    (0-31): 32 x Sequential(
      (0): Conv2d(256, 4, kernel_size=(1, 1), stride=(1, 1))
      (1): ReLU()
      (2): Conv2d(4, 4, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
      (3): ReLU()
      (4): Conv2d(4, 256, kernel_size=(1, 1), stride=(1, 1))
    )
  )
)
```

5




```
import matplotlib.pyplot as plt
import numpy as np


"""
Step 1 : Generate Toy data
"""

d = 35
n_train, n_val, n_test = 300, 60, 30
np.random.seed(0)
beta = np.random.randn(d)
beta_true = beta / np.linalg.norm(beta)
# Generate and fix training data
X_train = np.array([np.random.multivariate_normal(np.zeros(d), np.identity(d)) for _ in range(
                                                n_train)])
Y_train = X_train @ beta_true + np.random.normal(loc = 0.0, scale = 0.5, size = n_train)
# Generate and fix validation data (for tuning lambda).
X_val = np.array([np.random.multivariate_normal(np.zeros(d), np.identity(d)) for _ in range(
                                                n_val)])
Y_val = X_val @ beta_true
# Generate and fix test data
X_test = np.array([np.random.multivariate_normal(np.zeros(d), np.identity(d)) for _ in range(
                                                n_test)])
Y_test = X_test @ beta_true


"""
Step 2 : Solve the problem
"""

lambda_list = [2 ** i for i in range(-6, 6)]
num_params = np.arange(1,1501,10)

errors_opt_lambda = []
errors_fixed_lambda = []
for p in num_params :
    W = np.random.randn(p, d) / np.sqrt(p)

    # ReLU function
    X_train_transformed = np.maximum(X_train @ W.T, 0)
```

```python
    X_val_transformed = np.maximum(X_val @ W.T, 0)
    X_test_transformed = np.maximum(X_test @ W.T, 0)

    # (X^TX + lambda I_p)theta = X^TY : normal equation
    theta_fixed_lambda = np.linalg.solve(X_train_transformed.T @ X_train_transformed + 0.01 *
                                            np.eye(p), X_train_transformed.T @ Y_train)
    errors_fixed_lambda.append(np.mean((X_test_transformed @ theta_fixed_lambda - Y_test) ** 2
                                            ))

    val_errors = []
    for lambda_ in lambda_list:
        theta_opt_lambda = np.linalg.solve(X_train_transformed.T @ X_train_transformed +
                                                lambda_ * np.eye(p),
                                                X_train_transformed.T @ Y_train)
        val_errors.append(np.mean((X_val_transformed @ theta_opt_lambda - Y_val) ** 2))
    optimal_lambda = lambda_list[np.argmin(val_errors)]
    theta_opt_lambda = np.linalg.solve(X_train_transformed.T @ X_train_transformed +
                                            optimal_lambda * np.eye(p),
                                            X_train_transformed.T @ Y_train)
    errors_opt_lambda.append(np.mean((X_test_transformed @ theta_opt_lambda - Y_test) ** 2))
"""
Step 3 : Plot the results
"""

plt.figure(figsize = (24, 8))
plt.rc('text', usetex = True)
plt.rc('font', family = 'serif')
plt.rc('font', size = 24)


plt.scatter(num_params, errors_fixed_lambda, color = 'black',
            label = r"Test error with fixed $\lambda = 0.01$",
            )
plt.legend()

plt.plot(num_params, errors_opt_lambda, 'k', label = r"Test error with tuned $\lambda$")
plt.legend()
plt.xlabel(r'$\#$ parameters')
plt.ylabel('Test error')
plt.title(r'Test error vs. $\#$ params')

plt.savefig('double_descent.png')
plt.show()
```