

- REPORT : “Neural Network and Deep Learning”
 - 23300200022 滕勇功
 - Due to 8:00 AM, May 1, 2025.
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model & codes & dataset link :

- https://github.com/tyyyyyy333/Fdu_DS_DL24spring_collection/tree/main/project1

1. Project Overview

This project aims to implement a simple neural network framework using NumPy from scratch, and to train it on the MNIST dataset for image classification.

2. Implement Details

2.1 General MLP Structure:

$$\underbrace{Linear(m, n)}_{\text{customised}}$$

$$\rightarrow activation('ReLU', 'Sigmoid', 'LeakyReLU')$$

$$- > \text{Linear}(n_k, 10) - > \text{Loss_fn}$$

where m, n refer to units-in, units-out

2.2 CNN:

$$\begin{aligned}
 & \underbrace{\text{Conv2D}(m, n, k, o, p, q)}_{\text{customized}} \\
 & - > \text{activation}(\text{'ReLU'}, \text{'Sigmoid'}, \text{'LeakyReLU'}) \\
 & \quad - > \text{flatten} \\
 & \quad - > \underbrace{\text{Linear}(m^*, n^*)}_{\text{customized}} \\
 & - > \text{activation}(\text{'ReLU'}, \text{'Sigmoid'}, \text{'LeakyReLU'}) \\
 & \quad - > \text{Linear}(n_k, 10) - > \text{Loss_fn}
 \end{aligned}$$

where m, n, k, o, p, q respectively refer to the inchannel, outchannel, kernel_size, strides, paddings

2.3 Implement and Derivation:

2.3.1 Linear:

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial y} \frac{\partial y}{\partial x} = \text{grads} \cdot W^T$$

$$\frac{\partial L}{\partial W} = \frac{\partial L}{\partial y} \frac{\partial y}{\partial W} = x^T \cdot \text{grads}$$

$$\frac{\partial L}{\partial b} = \frac{\partial L}{\partial y} \frac{\partial y}{\partial b} = \text{grads}$$

- Here comes the codes:

🔍 | 解释 | 添加注释 | ×

```
def backward(self, grad : np.ndarray):    "ndarray": Unknown word.
```

```
"""
```

```
input: [batch_size, out_dim] the grad passed by the next layer.
```

```
output: [batch_size, in_dim] the grad to be passed to the previous layer.
```

```
This function also calculates the grads for W and b.
```

```
"""
```

```
self.grads['W'] = np.dot(self.input.T, grad) / self.input.shape[0]
```

```
self.grads['b'] = np.sum(grad, axis=0, keepdims=True) / self.input.shape[0]
```

```
#print(self.input.T.shape, grad.shape)
```

```
#print('-----')
```

```
out = np.dot(grad, self.W.T)
```

```
return out
```

🔍 | 解释 | 添加注释 | ×

```
def clear_grad(self):
```

```
    self.grads = {'W' : None, 'b' : None}
```

2.3.2 CNN:

$$\frac{\partial L}{\partial X} = \sum_{o=1}^{C_{out}} \delta_o \star \text{rot180}(W_o)$$

$$\frac{\partial L}{\partial W^{(o)}} = \sum_{n=1}^N \sum_{i,j} \delta_o^{(n)}(i,j) \cdot X_{[:,i:i+K,j:j+K]}^{(n)}$$

$$\frac{\partial L}{\partial b_o} = \sum_{n=1}^N \sum_{i,j} \delta_o^{(n)}(i,j)$$

- Here comes the codes:

```

grads = [batch_size, out_channel, new_h, new_w]
"""

batch_size = grads.shape[0]
X = self.input

self.grads['W'] = np.zeros_like(self.W_)
self.grads['b'] = np.zeros_like(self.b_)
dX = np.zeros_like(X, dtype=np.float64)

for i in range(grads.shape[2]):
    for j in range(grads.shape[3]):
        h_start = i * self.stride
        h_end = h_start + self.kernel_size
        w_start = j * self.stride
        w_end = w_start + self.kernel_size

        X_window = X[:, :, h_start:h_end, w_start:w_end]

        for o in range(grads.shape[1]):
            delta = grads[:, o, i, j][:, None, None, None]
            self.grads['W'][o] += np.sum(delta * X_window, axis=0)
            self.grads['b'][0, o, 0, 0] += np.sum(grads[:, o, i, j])
            dX[:, :, h_start:h_end, w_start:w_end] += delta * self.W_[o]

self.grads['W'] /= batch_size
self.grads['b'] /= batch_size

if self.padding > 0:
    dX = dX[:, :, self.padding:-self.padding, self.padding:-self.padding]

return dX

```

2.3.3 flatten:

To flatten the feature map into***[batch_size, features]*** shape to calculate by linear layer.

- Here comes the codes:

```

grads = [batch_size, out_channel, new_h, new_w]
"""

batch_size = grads.shape[0]
X = self.input

self.grads['W'] = np.zeros_like(self.W_)
self.grads['b'] = np.zeros_like(self.b_)
dX = np.zeros_like(X, dtype=np.float64)

for i in range(grads.shape[2]):
    for j in range(grads.shape[3]):
        h_start = i * self.stride
        h_end = h_start + self.kernel_size
        w_start = j * self.stride
        w_end = w_start + self.kernel_size

        X_window = X[:, :, h_start:h_end, w_start:w_end]

        for o in range(grads.shape[1]):
            delta = grads[:, o, i, j][:, None, None, None]
            self.grads['W'][o] += np.sum(delta * X_window, axis=0)
            self.grads['b'][0, o, 0, 0] += np.sum(grads[:, o, i, j])
            dX[:, :, h_start:h_end, w_start:w_end] += delta * self.W_[o]

self.grads['W'] /= batch_size
self.grads['b'] /= batch_size

if self.padding > 0:
    dX = dX[:, :, self.padding:-self.padding, self.padding:-self.padding]

return dX

```

2.3.4 MutiCrossEntropy:

softmax : $\hat{y}_i = \frac{e^{z_i - z_{\max}}}{\sum_{j=1}^n e^{z_j - z_{\max}}}$

- forward:

$$L = -\frac{1}{B} \sum_{j=1}^B \sum_{i=1}^{n_{class}} y_i^j * \log(\text{softmax}(y_i^j) + \epsilon)$$

- backward:

$$\frac{\partial L}{\partial y_i} = \frac{1}{B} \sum_{j=1}^B (\text{softmax}(y_i^{(j)}) - y_i^{(j)})$$

- Here comes the codes:

```
def forward(self, predicts, labels):
    """
    predicts: [batch_size, D]
    labels : [batch_size, ]
    This function generates the loss.
    """
    # / ---- your codes here ----/

    self.labels = labels
    if self.has_softmax:
        self.pred = softmax(predicts)
    else:
        self.pred = predicts
    one_hot = np.eye(self.max_classes)[self.labels]
    eps = 1e-8
    loss = -np.mean(np.sum(one_hot * np.log(self.pred + eps), axis=1))

    return loss

def backward(self):
    # first compute the grads from the loss to the input
    # / ---- your codes here ----/
    one_hot = np.eye(self.max_classes)[self.labels]
    self.grads = (self.pred - one_hot)
    # Then send the grads to model for back propagation
    self.model.backward(self.grads)

def cancel_soft_max(self):
    self.has_softmax = False
    return self
```

2.3.5 sigmoid:

$$\text{sigmoid}(x) = \frac{1}{1 + e^{-x}}$$

- backward:

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial y} \frac{\partial y}{\partial x} = grads * y * (1 - y)$$

- Here comes the codes:

```
return self.forward(x)

解释 | 添加注释 | ×
def forward(self, x):
    self.input = x
    output = 1 / (1 + np.exp(-x))
    return output

解释 | 添加注释 | ×
def backward(self, grads):
    assert self.input.shape == grads.shape
    y = self.forward(self.input)

    output = grads * y * (1 - y)
    return output
```

2.3.6 Other functions' implement codes:

- L2 penalty:

```
解释 | 添加注释 | ×
def forward(self, loss):
    w_sum = 0
    for layer in self.model.layers:
        if layer.optimizable:
            w_sum += np.sum(layer.params['W']**2)
    loss += self.lambda_ * w_sum
    return loss
```

- backward of L2 Loss:

```

↵ | 解释 | 添加注释 | ×
def forward(self, predicts, labels):
    if self.one_hot:
        self.labels = np.eye(self.max_classes)[labels]
    else:
        self.labels = labels

    if self.has_softmax:
        self.pred = softmax(predicts)
    else:
        self.pred = predicts

    loss = np.mean((self.pred - self.labels)**2)

    return loss

↵ | 解释 | 添加注释 | ×
def backward(self):
    self.grads = 2 * (self.pred - self.labels)
    self.model.backward(self.grads)

```

3. Experiment Setup

- learning rate : 1e-3 (default)
- optimizer : Adam / Momentum SGD / SGD (default)
- learning rate scheduler : None(default) / MultiStep / Exponential
- scaler : min-max-scaler
- loss function : MultiCrossEntropy(default) / MseLoss
- batch size : 128(default)
- dataset : Mnist
- random seed : 309
- running epoch : 10
- Weight decay : shut down(default)

4. Result

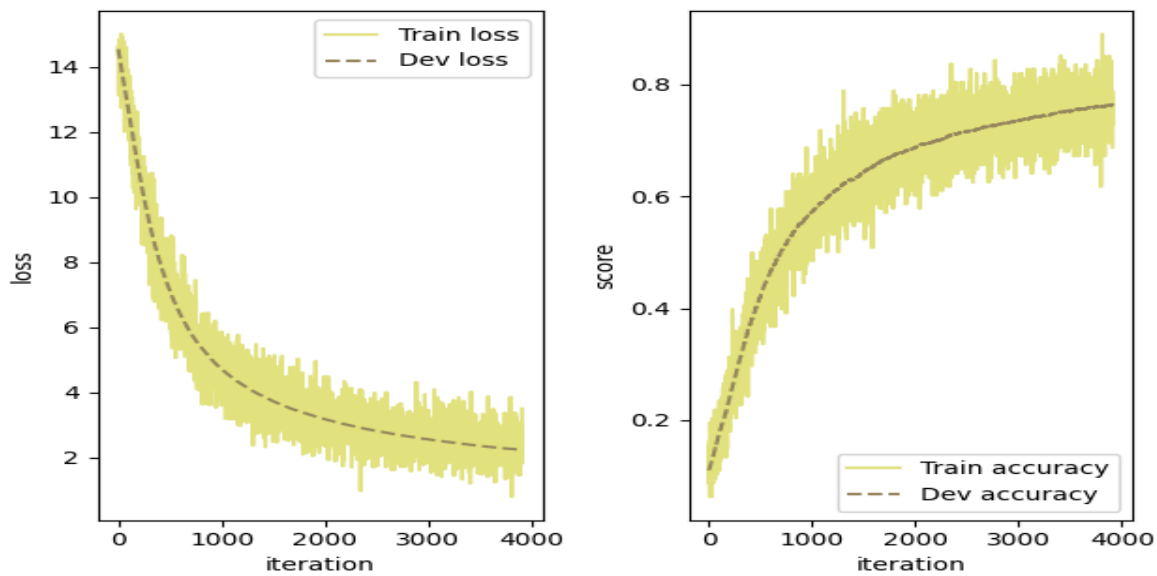
Unless otherwise specified, all the following results are obtained from the default settings in 3.

4.1 MLP

4.1.1 Metrics:

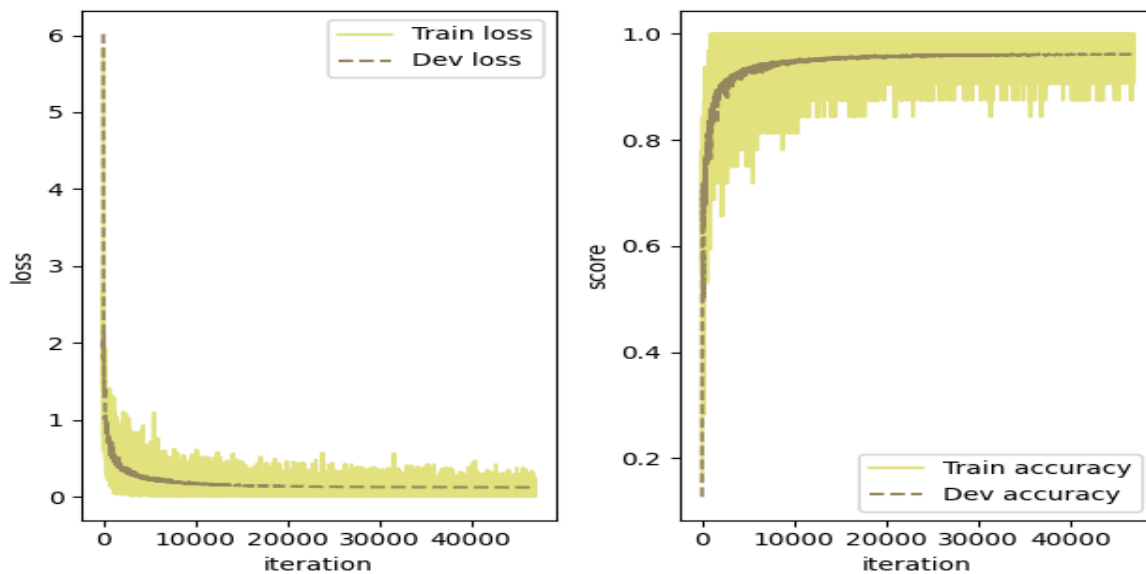
Defaulted setting

- valid Accuracy: 0.7634
- valid loss: 2.234
- loss graph as follows:



Developed setting

- valid Accuracy: 0.9535
- valid loss: 0.1541
- Setting seen in Appendix.
- loss graph as follows:

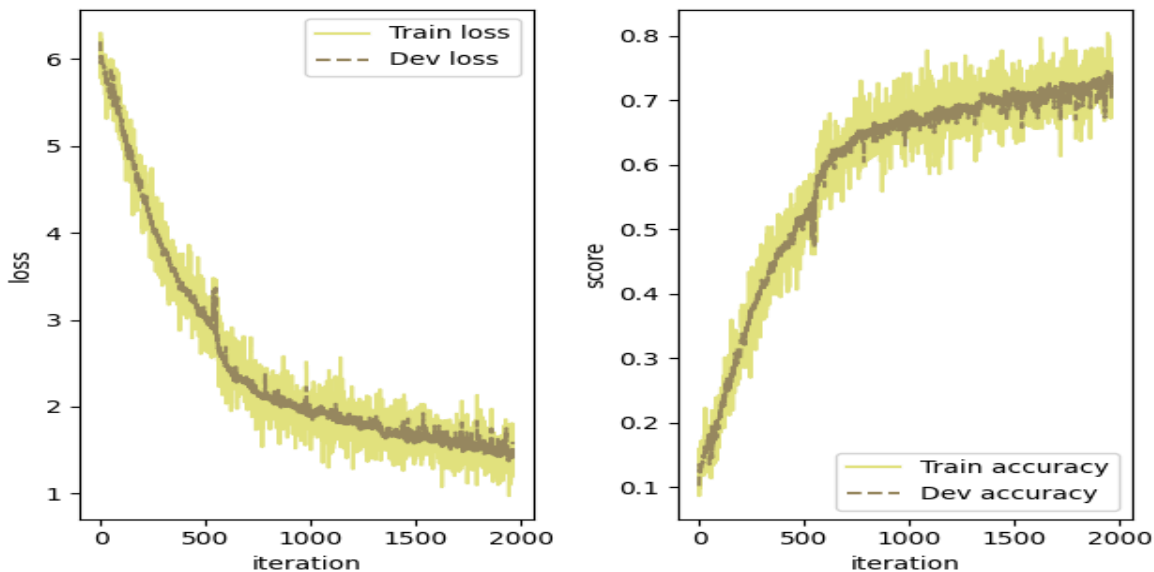


4.2 CNN

4.2.1 Metrics:

Defaulted setting

- Note : The accuracy can be worse than mlp when the cnn model is not well trained and designed.
- valid Accuracy: 0.7023
- valid loss: 1.5977
- loss graph as follows:



4.2.2 A note for the result of cnn:

Due to the efficiency of the CNN layer implementation, this CNN model cannot achieve too many and too deep cnn kernel settings(seen as Appendix). Similarly, the operation time required to ensure convergence is also too long. Therefore, the accuracy is lower than that of MLP. Under ideal conditions, CNN can carry more economical parameters, and the training effect should be better than MLP ideally.

4.3 Result of changing hyperparameters:

For convenience, following experiments are based on the defaulted MLP model to save the calculating time. Both defaulted details of MLP and CNN will be written in Appendix.

4.3.1 modifying layers:

Modify the layer units into {[784,500,100,10], [784,100,10], [784,500,10]}

while shut down the weight decay.

The activations are all 'ReLU' and the loss function is 'MultiCrossEntropy'.

[784,500,100,10] :

valid accuary : 0.8541

valid loss : 1.8914

[784,100,10] :

```
valid accuracy : 0.6799
valid loss : 1.967
```

```
[784,500,10] :
valid accuracy : 0.7898
valid loss : 2.262
```

4.3.2 learning rate:

Modify the learning rate into {1e-4, 1e-2, 1, 10}
using the lr_scheduler of 'MultiStep', 'Exponential' and 'None'.
All the valid accuracy and loss are based on the final epoch.

```
[1e-4, None] :
valid accuracy : 0.3678
valid loss : 8.1202
```

```
[1e-2, None] :
valid accuracy : 0.8898
valid loss : 0.7872
```

```
[1, None] :
valid accuracy : 0.9584
valid loss : 0.1660
```

Here the training accuracy is around 0.95

```
[10, None] :
valid accuracy : 0.0998
valid loss : 2.3954
```

```
[1, MultiStep] :
The milestones are [1000, 2000] and the gamma is 0.1
valid accuracy : 0.9439
valid loss : 0.2012
```

However, the lowest training loss is around 0.05 and the training accuracy is nearly 0.98

```
[1, Exponential] :
THE gamma is 0.999 and the lowest learning rate is 1e-5
valid accuracy : 0.8558
valid loss : 1.8909
```

However, the lowest training loss is around 0.08 and the training accuracy is nearly 0.98

4.3.3 optimizers:

Modify the optimizer into {'Adam', 'Momentum SGD', 'SGD'}
learning rate is 1e-3 as defaulted.

```
SGD :
valid Accuracy: 0.7634
valid loss: 2.234
```

Momentum SGD :

```
The mu is 0.9.
valid Accuracy: 0.7644
```

```
valid loss: 2.2335
```

Adam :

The beta_1 is 0.9, beta_2 is 0.999, epsilon is 1e-8.

```
valid Accuracy: 0.9327
```

```
valid loss: 0.4679
```

Actually, losses optimized by SGD and MomentumGD are not converged because of learning rate.

The Adam optimizer is the best one among them, for its self-adapting learning rate.

4.3.4 batch size:

Modify the batch size with {32, 128, 512}

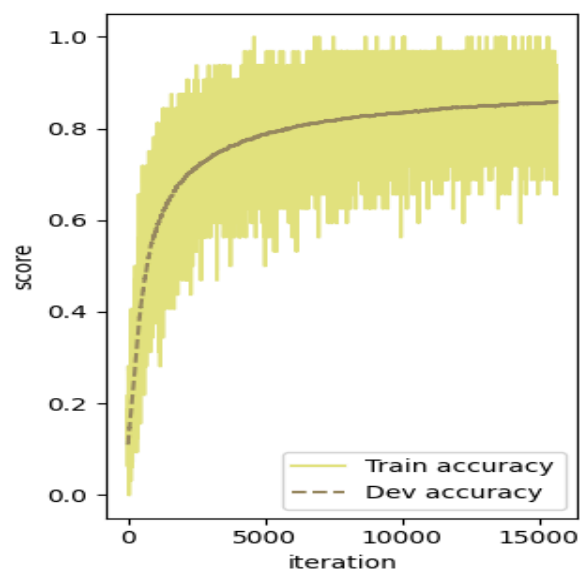
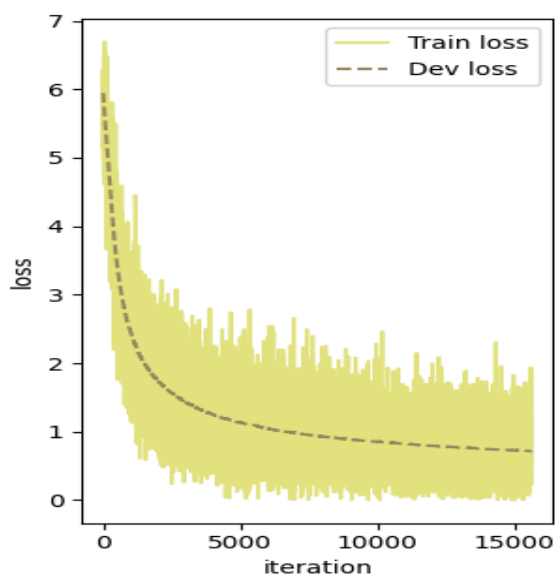
others are defaulted

32 :

```
valid Accuracy: 0.8573
```

```
valid loss: 0.7167
```

Here comes the loss tendency:



256(Defaulted) :

```
valid Accuracy: 0.7634
```

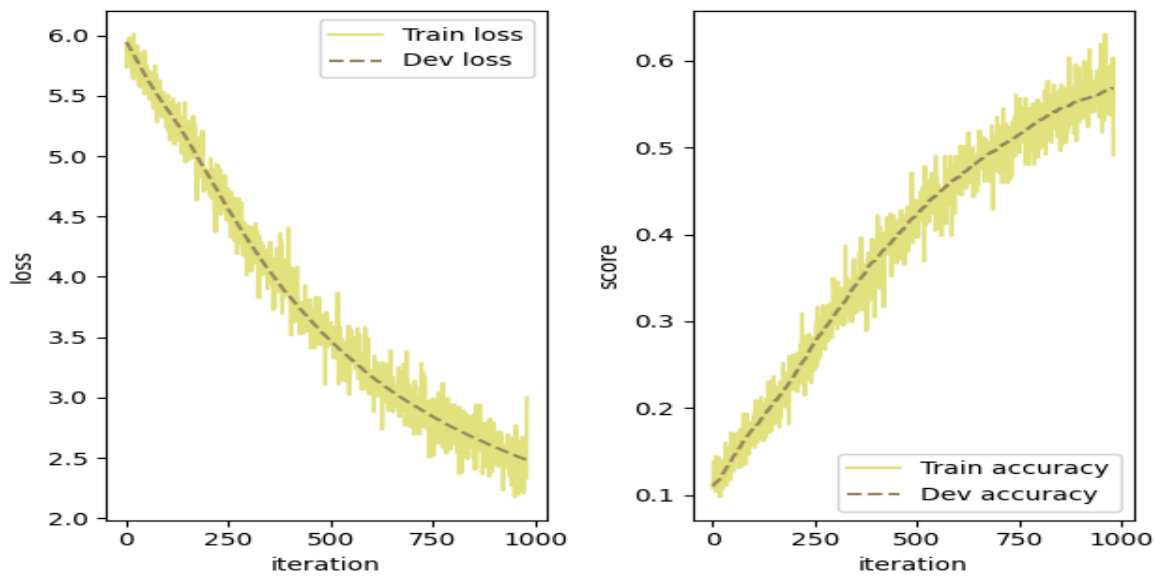
```
valid loss: 2.234
```

512 :

```
valid Accuracy: 0.5688
```

```
valid loss: 2.4836
```

Here comes the loss tendency:



The batch size of 32 is the best one, for it has the lowest loss and the highest accuracy.

The batch size of 512 is the worst one, for it has the highest loss and the lowest accuracy.

But with respect to the running time, the batch size of 512 is the best one, for it has the lowest running time.

4.3.5 loss_fn:

Modify the loss function with {'MultiCrossEntropy', 'MseLoss'}

others are defaulted

MultiCrossEntropy(Defaulted) :

valid Accuracy: 0.7634

valid loss: 2.234

MseLoss :

valid Accuracy: 0.7641

valid loss: 0.0426(mse)

4.3.6 data augmentation:

Modify the data augmentation a sequence of {'translate', 'rotate', 'random resize'}
Honestly, data augmentation is not so suited for MLP, but the manual CNN is too slow...

So here put the result as an illustration.

others are defaulted

with augmentation :

valid Accuracy: 0.6704

valid loss: 1.8192

without augmentation :

```
valid Accuracy: 0.6846
valid loss: 1.7559
```

4.3.7 regularization:

Modify the regularization with 'l2' , dropout, and weight_decay

others are defaulted

Consider that applying penalty may cause worse behavior, here we modify the learning rate to the best "1" as observed and apply the ExponentialLR with lowest lr of 1e-4. we modify the epoch to 20 for sufficient training.

with l2 :

The l2 lambda will be 1e-3

valid Accuracy: 0.9644

valid loss: 1.3579

with dropout :

The drop rate is 0.1

valid Accuracy: 0.8884

valid loss: 0.3245

This may be a potential issue.

Dropout essentially introduces the noise, which obstructs the convergence.

with weight_decay :

lambda will be 1e-3

valid Accuracy: 0.962

valid loss: 0.1277

defaulted :

valid Accuracy: 0.9442

valid loss: 0.1831

5.Error Analysis

5.1

The model is not accessible for the gradient update because of the following code: `layer.params[key] = layer.params[key] - self.init_lr * self.v[layer.layer_name][key]` in the `optimizer.py` due to the fact that the assignment creates a new object reference rather than modifying the original parameter in place.

As a result, the `layer.params[key]` in the model is disconnected from the optimizer's update mechanism.

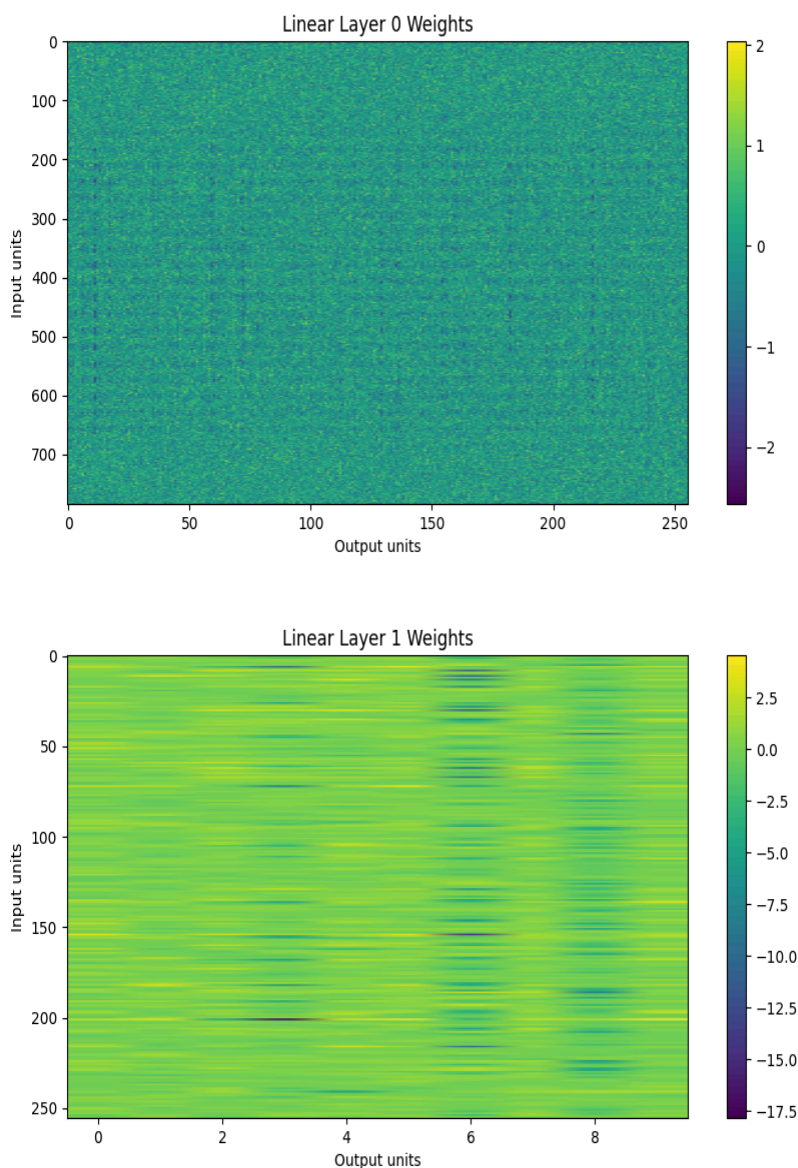
This leads to no actual parameter update during training, even though the gradients are correctly computed.

```
To fix this issue, the in-place update should be used instead: `layer.params[key] -=
self.init_lr * self.v[layer.layer_name][key]`
```

6.Feature Visualization

Here comes the visualization weight.

6.1 MLP:

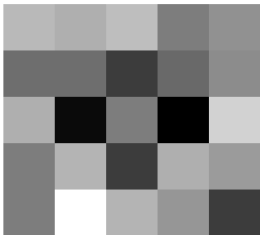


6.2 CNN:

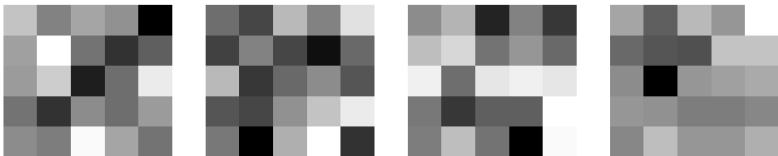
Here shows some visualization of the CNN kernels. A complete visualization of the kernels is too large to be displayed. So here we only show a few kernels of each

layer. Others will be uploaded in github.

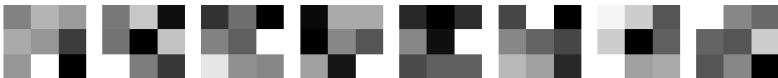
Conv Layer 0: Kernel 2

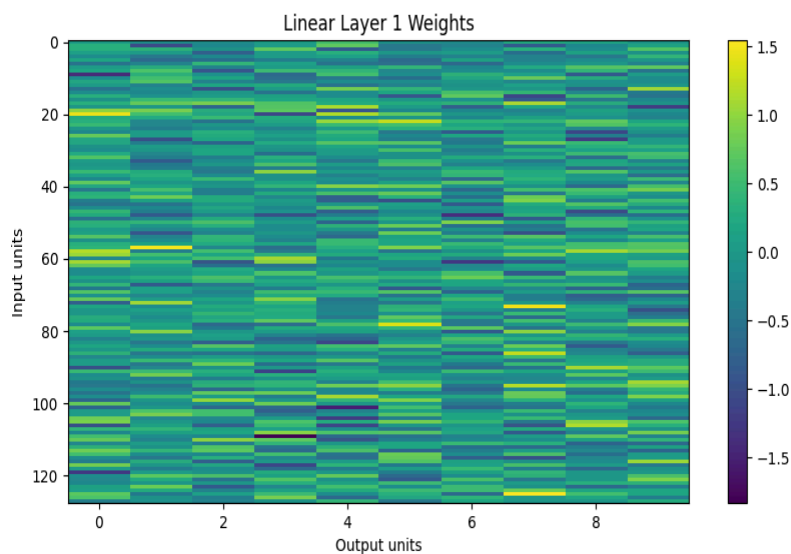
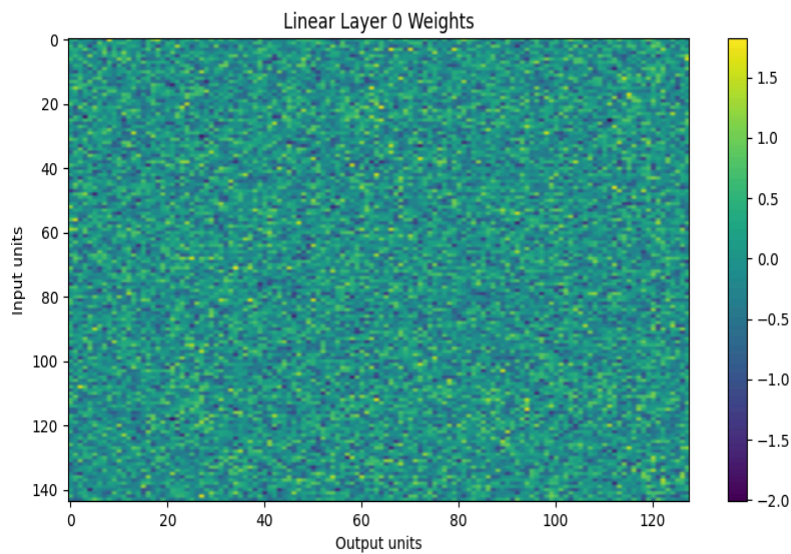


Conv Layer 1: Kernel 7



Conv Layer 2: Kernel 10





7. Conclusion

7.1. Comparison of Optimizers

* We compared several optimizers including SGD, SGD with momentum, and Adam. We found that Adam consistently provides faster convergence due to its adaptive learning rate mechanism, especially in the early stages of training. While SGD with momentum can also accelerate convergence, but it requires more careful tuning. Pure SGD, although simple, is more sensitive to the learning rate and generally slower. For our task, Adam achieved the best trade-off between speed and stability. *

7.2 Impact of Network Depth and Neurons

* Deeper networks or those with more neurons per layer have greater expressive power, but they are also more prone to overfitting and harder to train without regularization. In our experiments, increasing the number of hidden units in MLP

improved accuracy up to a point, after which diminishing returns. In contrast, deeper net is more effective for optimizing. *

7.3 Effectiveness of Regularization

* We applied both L2 regularization, dropout and weight decay to prevent overfitting. L2 and weight decay help to keep the weights from growing too large, while dropout forces the network to develop more robust, redundant representations. Both methods improve generalization, especially for MLPs, which otherwise easily overfit the MNIST dataset. However, excessive regularization can lead to underfitting, especially when using shallow networks. As a sample, dropout here plays a worse role in training for its offensive behavior, which is adding noise in essence. *

7.4 Benefits of Cross-Entropy Loss

* Using softmax combined with cross-entropy loss provided a probabilistic interpretation of the model's output and a smooth, numerically stable loss surface. We confirmed that this formulation simplifies gradient computation and ensures better class separation during training compared to mean squared error (MSE), which performed worse in early experiments due to less sharp gradient signals. (although we have not been observed the difference of training loss from mse yet in experiments...due to the fault of the configuration for hyperparameters) *

7.5 Convolutional Network Performance and Limitations

* The convolution layers are able to extract local and hierarchical patterns such as edges and textures, which the MLP could not learn effectively. However, our self-built CNN performs slightly worse than reference implementations, likely due to a limited number of convolutional filters. This constraint is imposed due to running time limitations for the CPU. A smaller number of filters restricts the network's feature representation capacity, especially in deeper layers. *

7.6 Insights from Visualization

* Visualizing the learned convolutional filters revealed that early layers typically detect edges or gradients, while deeper layers captured more abstract shapes. Feature map visualization helped confirm that the CNN progressively distilled the input image into more discriminative representations. *

7.7 Hyperparameter Tuning Effects

* Through systematic tuning of hyperparameters such as learning rate, batch size, number of filters, and dropout rate, we observed several important dynamics *:

- Too large a learning rate led to oscillations or divergence, while too small a rate slowed convergence significantly.
- Small batch sizes improved generalization but made the training process noisier.
- Increasing the number of filters or hidden units enhanced accuracy but also raised computational cost and overfitting risk.
- regularization methods helped regularize the model, but if set too high, harmed learning by removing too much information.

Overall Learning Outcome

* Building a deep learning model from scratch provided us with invaluable insights into the architecture and training mechanics of neural networks. We learned how each component—from activation functions to gradient updates—affects the final performance. While our CNN was relatively shallow and constrained by resources, the implementation process deepened our understanding of feature extraction, training dynamics, and model interpretability. This hands-on experience clarified not just the "how," but also the "why" behind deep learning models' behavior. *

8.Appendix

8.1 Details of MLP:

Default:

Linear 1 : (784, 256)

->ReLU 1

->Linear 2 : (256, 10)

->Softmax + MultiCrossEntropy

Default setting

Developed:

Linear 1 : (784, 512) weight_decay=0.001

->ReLU 1

->Linear 2 : (512, 256) weight_decay=0.001

->ReLU 2

->Linear 3 : (256, 10) weight_decay=0.001

->Softmax + MultiCrossEntropy

```
learning_rate = 1e-1
batch_size = 32
epochs = 15
optimizer = MomentumGD
lr_scheduler = ExponentialLR(gamma=0.9999,lowest_lr=7e-4)
```

8.2 Details of CNN:

Default:

```
Conv 1 : (1 → 4), kernel_size=5, stride=2, padding=1
```

->ReLU

->Conv 2 : (4 → 8), kernel_size=5, stride=2, padding=1

->ReLU

->Conv 3 : (8 → 16), kernel_size=3, stride=2, padding=1

->ReLU

→Flatten

->Linear 1 : (16 * 3 * 3 → 128)

->ReLU

->Linear 2 : (128 → 10)

->Softmax + MultiCrossEntropy

Default setting

8.3 statement of scores and weight availability

Consider that multiple parameters change in the experiment, the model weights in the netdisk or github will be reserved only for a basic version and a seemingly best one(only for mlp...) as declaration of model availability, and all the valid scores documented in this markdown are the behavior for the final epoch of a training process, rather than representing the behavior of the model weight, which documents the best one. All the setting will be defaulted unless declaring.