MINI PROJECT II: IMPLEMENTATION OF PYTORCH MODULES

1 Implementation of Modules: Base class

All Modules in our implementation are based on the following base class `Module` structure:

```
class Module(object):
    def __init__(self) -> None:
        pass
    def forward(self, *input):
        raise NotImplementedError
    def backward(self, *gradwrtoutput):
        raise NotImplementedError
    def param(self):
        return []
    def to(self, device):
        return self
    def load_param(self, *param, device):
        return None
```

Listing 1: Base class.

- `param()` function returns the list of parameters in a module, e.g. for `Conv2d` and Upsampling, the parameters are `[(self.weight, self.dl_dw), (self.bias, self.dl_db)]`.
- `to(self, device)` function moves the module to the specified device, possible devices are `'cpu'` and `'cuda'`. We used `'cuda'` during training to increase matrix calculation speed (about 10$\sim$30$\times$ faster, takes about 5 second per epoch to train our models in Appendix 1).
- For each module, we also provide a `load_param(self, *param)` to load saved weights back to the modules.

2 Conv2d Module

The major tools we use in this implementation are: `torch.nn.functional.unfold/fold` and `torch.einsum` for multidimensional tensor multiplication. Here we illustrate the forward/backward pass of `Conv2d`.

The forward pass of our `Conv2d` module is in the following order:

1. **Reshape kernel weights**: $[C_{out}, C_{in}, ks, ks] \rightarrow [C_{out}, C_{in} \times ks^2]$.
   Where $C_{in/out}$ stands for numbers of in/output channels and ks stands for kernel_size.
2. **Unfold input tensor**: $[bz, C_{in}, H_{in}, W_{in}] \rightarrow [bz, C_{in} \times ks^2, H_{out} \times W_{out}]$.
   Where bz stands for batch size, and H, W stands for height and width of in/output images. The output of this step is saved in the model class as `self.unfolded` for later use in backpropagation. And the relationship between input and output widths and heights are (we assume hyperparameter inputs are `int` instead of `tuple`):

$$H_{out} = \left\lfloor \frac{H_{\text{in}} + 2 \times \text{ padding } - \text{ dilation } \times (\text{kernel\_size} - 1) - 1}{\text{stride}} + 1 \right\rfloor$$
$$W_{out} = \left\lfloor \frac{W_{\text{in}} + 2 \times \text{ padding } - \text{ dilation } \times (\text{kernel\_size} - 1) - 1}{\text{stride}} + 1 \right\rfloor$$

3. **Matrix Multiplication** $\mathbf{Y} = \mathbf{X}\mathbf{W} + \mathbf{b}$:
   $[bz, C_{in} \times ks^2, H_{out} \times W_{out}] \times [C_{out}, C_{in} \times ks^2] + [C_{out},] = [bz, C_{out}, H_{out} \times W_{out}]$.
4. **Reshape output**: $[bz, C_{out}, H_{out} \times W_{out}] \rightarrow [bz, C_{out}, H_{out}, W_{out}]$

The backward pass of our `Conv2d` module is in the following order:

1. **Reshape upstream gradients** $\partial \mathbf{L}/\partial \mathbf{Y}$: $[bz, C_{out}, H_{out}, W_{out}] \rightarrow [bz, C_{out}, H_{out} \times W_{out}]$.
2. **Reshape kernel weights**: $[C_{out}, C_{in}, ks, ks] \rightarrow [C_{out}, C_{in} \times ks^2]$.
3. **Apply chain rule** $\frac{\partial \mathbf{L}}{\partial \mathbf{X}} = \frac{\partial \mathbf{L}}{\partial \mathbf{Y}} \mathbf{W}^T$**:**
   $[bz, C_{out}, H_{out} \times W_{out}]^T [C_{out}, C_{in} \times ks^2] \xrightarrow{\texttt{einsum}} [bz, C_{in} \times ks^2, H_{out} \times W_{out}]$.
4. **Apply** `fold` **to recover shape of** $\frac{\partial \mathbf{L}}{\partial \mathbf{X}}$ **to** $\mathbf{X}$: $[bz, C_{in} \times ks^2, H_{out} \times W_{out}] \xrightarrow{\texttt{fold}} [bz, C_{in}, H_{in}, W_{in}]$.

5. **Acquire gradients w.r.t weights in** `self.unfolded` $\frac{\partial \mathbf{L}}{\partial \mathbf{W}} = \mathbf{X}^T \frac{\partial \mathbf{L}}{\partial \mathbf{Y}}$ **and transform to the original weight shape**:
   $[bz, C_{in} \times ks^2, H_{out} \times W_{out}]^T [bz, C_{out}, H_{out} \times W_{out}] \xrightarrow{\texttt{einsum}} [C_{out}, C_{in} \times ks^2] \rightarrow [C_{out}, C_{in}, ks, ks]$.
6. **Acquire gradients w.r.t bias:** $\frac{\partial \mathbf{L}}{\partial \mathbf{b}} = \frac{\partial \mathbf{L}}{\partial \mathbf{Y}}$:
   $[bz, C_{out}, H_{out}, W_{out}] \xrightarrow[\texttt{flatten}]{\texttt{transpose}} [C_{out}, bz \times H_{out} \times W_{out}] \xrightarrow{\texttt{mean}} [C_{out},]$.

In terms of initialization, we use the same method as in the `reset_parameters(self)` function in PyTorch repository. Entire implementation of `Conv2d` module is shown in Appendix 2.

3 Upsampling Module

In our implementation, the `Upsampling` module is implemented in the way of *nearest neighbor* sampling (NN Sample) + convolution. Two tricky parts in this implementation are: 1) implement nearest neighbor sampling efficiently, 2) implement backward gradient pass of nearest neighbor sampling.

In terms of nearest neighbor sampling, we implement it with `torch.repeat_interleave` as follows (simplified due to paragraph limit):

```
def nearest_neighbor_sampling(self, inp, scale_factor):
    inter = repeat_interleave(inp, repeats=scale_factor, dim=-1)
    ret = repeat_interleave(inter, repeats=scale_factor, dim=-2)
    return ret
```

Listing 2: Nearest neighbor sampling.

The back propagation of `Upsampling` consists of two parts: 1) backprop the upstream gradients from output to convolution layer input $\partial \mathbf{L}/\partial \mathbf{X}_{up}$, and 2) back prop from convolution input to input $\partial \mathbf{X}_{up}/\partial \mathbf{X}$ (passing the NN Sample module). Where 1) can simply be achieved by backpropagating the convolution layer in `Upsampling`, whereas, the second requires a special type of gradient accumulation way which depends on the `scale_factor` in the NN Sample part. An example of this type of accumulation is shown in Eq. (1) (with `scale_factor=2`):

$$\underbrace{\left[\begin{array}{cc|cc} 1 & 0 & 0 & 2 \\ -3 & 4 & 2 & 1 \\ \hline -2 & 0 & 0 & 1 \\ 0 & 3 & 0 & 1 \end{array}\right]}_{\partial \mathbf{L}/\partial \mathbf{X}_{up}} \rightarrow \underbrace{\begin{bmatrix} 2 & 5 \\ 1 & 2 \end{bmatrix}}_{\partial \mathbf{L}/\partial \mathbf{X}} \tag{1}$$

This is implemented with two for loops, we use tensor operations to accelerate on GPU:

```
def backward(self, grdwrtoutput):
    dl_dw = self.conv.backward(grdwrtoutput)
    N, C, H, W = dl_dw.size()
    out_h, out_w = H // self.scale_factor, W // self.scale_factor
    rows = arange(0, H, self.scale_factor).repeat(out_h)
    cols = arange(0, W, self.scale_factor).repeat_interleave(out_w)
    dl_dx = zeros(dl_dw[..., cols+0, rows+0].size()).to(grdwrtoutput.device)
    for i in range(self.scale_factor):
        for j in range(self.scale_factor):
            dl_dx = dl_dx + dl_dw[..., cols+i, rows+j]
    dl_dx = dl_dx.reshape(N, C, out_h, out_w)
    return dl_dx
```

Listing 3: Backprop of `Upsampling` module.

4 Nonlinearities

ReLU: `torch.clamp` and `torch.sign` are mainly used to implement `ReLU` module. Module implement main steps: clamp input $\rightarrow$ output 0 or input itself $\rightarrow$ sign input and then clamp $\rightarrow$ 1 or 0, notice this module has no parameters.

Sigmoid: `torch.exp` is used to implement `sigmoid` module with following equations. $\text{Sigmoid}(x) = \frac{1}{1+e^{-x}}$, $\text{Sigmoid'}(x) = \frac{(e^{-x}+1)-1}{1+e^{-x}} \frac{1}{1+e^{-x}} = (1 - \text{Sigmoid}(x))\,\text{Sigmoid}(x)$, this module also has no parameters.

5 Mean Squared Error Loss Function Module

`MSELoss` module is implemented with `torch.pow`, `torch.mean`, and `torch.size` with the following equations. $\text{MSELoss}(y,t) = \frac{1}{N}\sum_{i=0}^{N}(y_i - t_i)^2$, $\text{MSELoss'}(y,t) = \frac{2}{N}\sum_{i=0}^{N}(y_i - t_i)$, where N is total elements in y and t. The module does following things: initialize the prediction y and target $t \Rightarrow$ compute the loss and compute the gradient w.r.t prediction y.

6 Stochastic Gradient Descent optimizer Module

`SGD` module is mainly implemented with `torch.add` and `torch.Tensor.zero_`. `SGD` module has `zero_grad()` to set all grad parameters in the input parameters to 0, and `step()` to update grad parameters in the input parameters by `w += -grad * lr`.

7 Sequential Module

`Sequential` module needs to make sure that both forward inputs and backward gradients, as well as backward gradients, could flow smoothly during training. Moreover, `Sequential` module also needs to take care of gathering parameters from all sub modules and loading back the parameters to its sub modules. All these are done by:

```
class Sequential(Module):
    def __init__(self, *layers) -> None:
        super().__init__()
        self.modules = []
        for layer in layers:
            self.modules.append(layer)

    def forward(self, x):
        ret = x
        for layer in self.modules:
            ret = layer.forward(ret)
        return ret

    def backward(self, gradwrtoutput):
        grad_from_back = gradwrtoutput
        for layer in reversed(self.modules):
            grad_from_back = layer.backward(
     grad_from_back)
    def __call__(self, input):
        return self.forward(input)
```

Listing 4: `Sequential` functioning part.

```
def to(self, device):
    for i, module in enumerate(self.modules):
        self.modules[i] = module.to(device)
    return self
def param(self):
    ret = []
    for layer in self.modules:
        ret.append(layer.param()[0])
        if len(layer.param()) > 1:
            ret.append(layer.param()[1])
    return ret

def load_param(self, param):
    model_idx = param_idx = 0
    while model_idx < len(self.modules) and (param_idx < len(param)):
        required_length = len(self.modules[model_idx].param())
        self.modules[model_idx].load_param(param[param_idx:
      required_length+param_idx])
        param_idx += required_length
        model_idx += 1
```

Listing 5: Auxiliary: switch device save/load parameters.

8 Parameters Handling

The parameters throughout the framework are the group within tuples in the way of (`weight`, `grad`). The parameter saving process is done after transmitting all the parameters in the model to CPU in order to avoid device issues during the loading process. Two snippets of loading and saving are shown below:

```
def load_pretrained_model(self):
    print('Loading trained model from', self.
     default_model_dir)
    with open(self.default_model_dir, 'rb') as f:
        params = pickle.load(f)
    # model load params on self.device
    self.model.load_param(params, self.device)
    print('Model loaded.')
    return True
```

Listing 6: `load pretrained` Module part.

```
def save_model(self, dir):
    params = self.model.param()
    for i, tup in enumerate(params):
        tup2list = list(tup)
        for j, v in enumerate(tup2list): # move params to cpu
            if v is not None: tup2list[j] = v.to('cpu')
        params[i] = tuple(tup2list)
    with open(dir, 'wb') as f: pickle.dump(params, f)
    print('Model saved at: ', dir)
```

Listing 7: `Save` Module part.

Appendix 1: Experiment

In terms of experiment design, we implement several *Noise2Noise*-like model structures to test our modules' performance. Due to space limitations, we report validation performance on the given dataset of two typical models and their training curves as well as final visualizations.

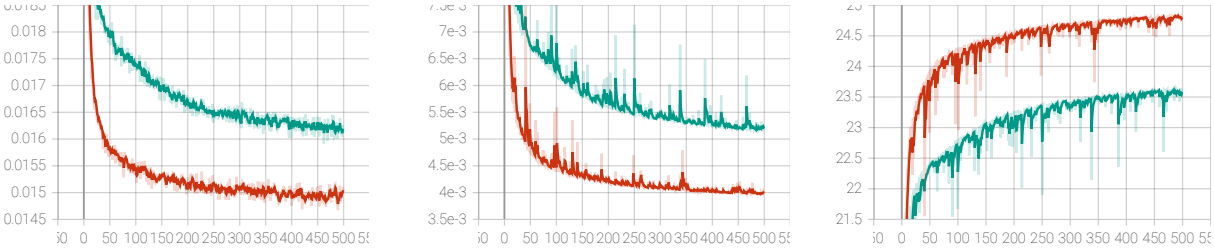
```
model = Sequential(
    Conv2d(3, 32, 3, stride=1),
    ReLU(),
    Conv2d(32, 64, 3, stride=1, padding=3),
    ReLU(),
    Upsampling(2, 64, 32, stride=2),
    ReLU(),
    Upsampling(2, 32, 3, stride=2),
    Sigmoid()
)
```

Listing 8: Best performance model 1.

```
model = Sequential(
    Conv2d(3, 32, 3, stride=2, padding=2),
    ReLU(),
    Conv2d(32, 64, 3, stride=2, padding=2),
    ReLU(),
    Upsampling(2, 64, 32, kernel_size=4, stride=1),
    ReLU(),
    Upsampling(2, 32, 3, stride=1, kernel_size=3),
    Sigmoid()
)
```

Listing 9: Model 2: Conv2d stride 2.

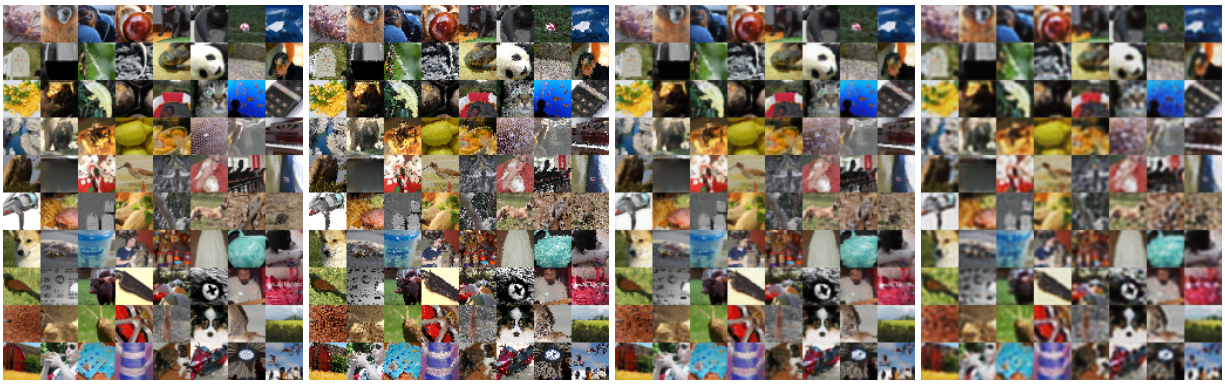
We trained both models for 500 epochs with batch size 16 and SGD of learning rate 8e-2. The best performances they achieved were **24.84dB** for model 1 and **23.64dB** for model 2 (we submitted model 2 as per requirements). We believe by training more epochs we could achieve slightly even better results, but this result is already convincing for the performance of our self-implemented modules. The training/validation curves are shown in Fig. 1.



(a) Training loss (MSE). (b) Validation Loss (MSE). (c) Validation PSNR.

Figure 1: Training/Validation curves of Model 1 and Model 2.

The result visualizations are shown in Fig. 2. From the results, we can see that the image output from model 1 is slightly sharper than the image output from model 2, but they both perform well in removing salt and pepper noise from the original input.



(a) Ground truth image (b) Input noisy image (c) Model 1 output (d) Model 2 output

Figure 2: Visualization results at validation.

Appendix 2: Conv2d Implementation

```
class Conv2d(Module):
    def __init__(self, in_channels, out_channels, kernel_size=3, bias=True, dilation=1, stride=1, padding=0):
        self.in_channels = in_channels
        self.out_channels = out_channels
        self.kernel_size = kernel_size
        self.dilation = dilation
        self.stride = stride
        self.padding = padding
        self.use_bias = bias

        # torch initialization
        n = in_channels * kernel_size**2
        stdv = 1. / math.sqrt(n)

        self.weight = empty(out_channels, in_channels, kernel_size, kernel_size).uniform_(-stdv, stdv)
        self.bias  = empty(out_channels).uniform_(-stdv, stdv)
        self.dilation = dilation
        self.padding = padding
        self.stride = stride
        self.unfolded = None
        self.x = None

        # gradient
        self.dl_dw = empty(self.weight.size())
        self.dl_db = empty(self.bias.size())

    def forward(self, x):
        self.x = x
        self.unfolded = unfold(x, kernel_size = self.kernel_size, dilation=self.dilation, padding=self.padding, stride=self.
     stride)
        weight = self.weight.reshape(self.out_channels, -1)
        wxb = einsum('ow,bws->bso', weight, self.unfolded)
        if self.use_bias:
            wxb += self.bias
        wxb = einsum('bso->bos', wxb)
        out_h = math.floor((x.shape[-2] - (self.kernel_size-1)*self.dilation + 2*self.padding - 1) / self.stride + 1)
        out_w = math.floor((x.shape[-1] - (self.kernel_size-1)*self.dilation + 2*self.padding - 1)  / self.stride + 1)

        #ret = fold(wxb, output_size=(out_h, out_w), kernel_size=(1,1))
        ret = wxb.reshape(-1, self.out_channels, out_h, out_w)
        return ret

    def backward(self, grdwrtoutput):
        grdwrtoutput = grdwrtoutput.flatten(2, -1)
        weight = self.weight.reshape(self.out_channels, -1)
        # here x is cin*kernelsize^2 and s is Hout*Wout
        dl_dx = einsum('ox,nos->nxs', weight, grdwrtoutput)
        out_size = (self.x.size(-2), self.x.size(-1))
        dl_dx = fold(dl_dx, output_size=out_size, kernel_size=self.kernel_size, dilation=self.dilation, padding=self.padding,
     stride=self.stride)

        self.dl_dw.add_(einsum('nos,nxs->ox', grdwrtoutput, self.unfolded).reshape(self.weight.size()))
        self.dl_db.add_(grdwrtoutput.transpose(0, 1).flatten(1, -1).mean(1))
        return dl_dx

    def param(self):
        return [(self.weight, self.dl_dw), (self.bias, self.dl_db)]

    def __call__(self, input):
        return self.forward(input)

    def to(self, device):
        self.dl_dw = self.dl_dw.to(device)
        self.dl_db = self.dl_db.to(device)
        self.weight = self.weight.to(device)
        self.bias = self.bias.to(device)
        return self

    def load_param(self, param, device):
        self.weight, _ = param[0]
        self.bias, _ = param[1]
        self = self.to(device)
```

Listing 10: Implemetation of `Conv2d`.