Hands-on Introduction to Deep Learning with PyTorch

More on Training Deep Learning Models

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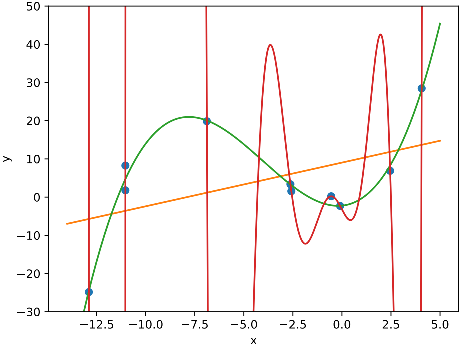
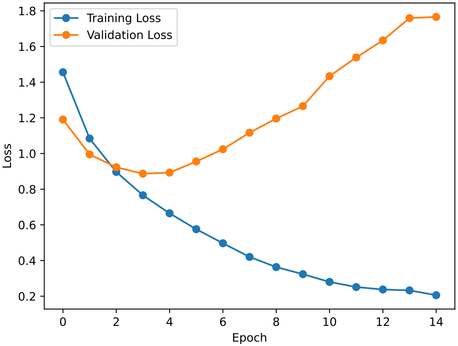
Overfitting

Overfitting happens when the model is too complex (compared to the noisiness of the training data)



Overfitting



- Low training loss
- High validation loss
- Large gap: generalization error
- The model performed better early on

Early Stopping

Stop training when the validation error reaches a minimum.

An trivial implementation of early stopping is to save the best model.

PyTorch: State Dictionary

- Learnable parameters (weights, biases) are stored in `torch.nn.Module`'s parameters
  - `module.parameters()`
- A state dictionary maps each layer of the model to the corresponding parameter
  - `model.state_dict()`
- Optimizers (`torch.optim`) also have a state dictionary
  - Useful to resume training

PyTorch: Save and Load Parameters to File

```
model = ...
optimizer = ...

torch.save(
  model.state_dict(), PATH
)
torch.save(
  optimizer.state_dict(), PATH
)
```

```
model = ...
optimizer = ...

model.load_state_dict(
  torch.load(PATH)
)
optimizer.load_state_dict(
  torch.load(PATH)
)
```

Convention: use `.pt` or `.pth` file extensions.

PyTorch: Save and Load Parameters

- `state_dict()` returns a reference to the state dictionary
- Use `deepcopy` to copy the state dictionary

```
model = ...

best_model_state = deepcopy(model.state_dict())
```

Regularisation: Loss Funtion

Add constraints on the model (model weights) via the loss function

PyTorch: L_2 Regularization

$$L_2 = \lambda \sum_i w_i^2$$

L_2 loss is quite common, and easily available in PyTorch via the `weight_decay` parameter in various optimizers (`SGD`, `Adam`, ...)

PyTorch: L_1 Regularization

L_1 regularization often produces a sparse model (many weights close to or equal to 0)

$$L_1 = \lambda \sum_i |w_i|$$

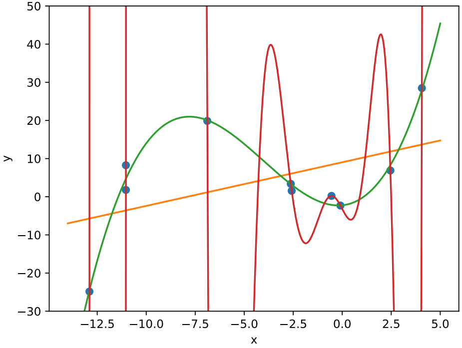
```python
def l1_loss(params, lambda):
    l1 = 0
    for p in params:
      l1 += torch.sum(torch.abs(p))

    return lambda * l1

total_loss = loss + l1_loss(model.parameters(), lambda = 0.01)
total_loss.backward()
```

Regularization: Reduce Model Capacity

Reducing the model capacity (number of parameters) can reduce over-fitting.




```python
# Compute number of parameters

num_elements_list = [
  p.numel()
  for p in model.parameters()
  if p.requires_grad
]

sum(num_elements_list)
```

Regularization: Dropout Layers

- Randomly zero some elements of the input with probability p
  - Each channel zeroed out independently
- Outputs scaled by $(1-p)^{-1}$
- Prevents co-adaptation of neurons

Monte Carlo Dropout for Error Estimation

- Perform multiple predictions with dropouts
  - Only have dropout layers in `train()` mode
- Average predictions
- Standard deviation is also available

```
y_all = np.stack([
  model(x).cpu().numpy()
  for i in range(n)
])

y = np.mean(y_all, axis=0)
```

```
def enable_dropout(model):
  for m in model.modules():
    mname = m.__class__.__name__
    if mname.startswith('Dropout'):
      m.train()
```

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If you finish the exercises early, try to implement Monte Carlo Dropout

Data Augmentation

Data augmentation artificially inflates the size of the training set by transforming the data (on-the-fly) at each iteration

- Random rotations
- Random translations
- Random re-sizing and clipping
- Random flips
- ...

Data augmentation helps reducing overfitting

PyTorch: Data Augmentation with torchvision's transforms (V1)

```python
from torchvision import transforms

transform = transforms.Compose([
  transforms.ToTensor(), # Deprecated in V2
  transforms.RandomResizedCrop(),
  transforms.RandomHorizontalFlip(),
  # ...
  transforms.Normalize(
    mean=[0.485, 0.456, 0.406], std=[0.229, 0.224, 0.225]
  ),
])
```

https://pytorch.org/vision/stable/transforms.html

Adaptive Learning Rate

- A fixed learning rate might not be optimal for the whole training
- The learning rate can be adjusted during training
  - Based on the number of epochs
  - Based on some validation metrics (`ReduceLROnPlateau`)

PyTorch: Learning Rate Scheduler

PyTorch's `torch.optim.lr_scheduler` provides several methods/policies to adjust the learning rate.

```
optimizer = optim.SGD(model.parameters(), lr=0.01, momentum=0.9)
scheduler = ExponentialLR(optimizer, gamma=0.9)

for epoch in range(20):
    for input, target in dataset:
        optimizer.zero_grad()
        output = model(input)
        loss = loss_fn(output, target)
        loss.backward()
        optimizer.step()
    scheduler.step()
```

https://pytorch.org/docs/stable/optim.html

Optimizers

SDG takes small, regular steps

$$\theta_t = \theta_{t-1} - \eta \nabla_{\theta_{t-1}} \mathcal{L}(\theta_{t-1})$$

Momentum optimization:

$$\mathbf{m}_t = -\eta \nabla_{\theta_{t-1}} \mathcal{L}(\theta_{t-1}) - \beta \mathbf{m}_{t-1}$$

$$\theta_t = \theta_{t-1} + \mathbf{m}_t$$

Weights Initialisation

- Weights are randomly initialized
  - Uniform
  - Normal
  - ...
- Initialization has an impact on training
- Sensible choices of random distribution by default

https://xkcd.com/1838

PyTorch: Weights Initialisation

```python
def custom_weights_init(module):
    if isinstance(module, nn.Linear):
        module.weight.data.normal_(mean=0.0, std=1.0)
        if module.bias is not None:
          module.bias.data.zero_()

    if isinstance(module, nn.Conv2D):
        # Use torch.nn.init module
        torch.nn.init.xavier_uniform_(module.weight.data)

model.apply(custom_weights_init)
```

Transfer Learning and Fine Tuning: Motivation

- Training a deep learning model can be very expensive
- Many tasks are closely related
- Some data sets are too small to train a performant deep learning model
- Random initialization is far from optimal

Transfer learning and fine tuning aim at re-using pre-trained models and fine tune them for the specific task at hand.

Transfer Learning and Fine Tuning: CNN Example

CNNs for classification have two conceptual building blocks:

- Feature extractor (convolution layers)
- Classifiers (linear layers)

Feature extraction layers can be re-used from successfully trained models, while the classifier can be re-trained for the task at hand.

PyTorch: Load TorchVision Pre-Trained Models

```python
from torchvision.models import resnet50, ResNet50_Weights

resnet50(weights=ResNet50_Weights.IMAGENET1K_V2)

resnet50(weights=ResNet50_Weights.DEFAULT)

resnet50(weights="IMAGENET1K_V2")

# No weights (random initialization)
resnet50(weights=None)
```

PyTorch Hub

PyTorch Hub supports publishing pre-trained models!

```
# hubconf.py (on GitHub)
dependencies = ['torch']

def my_model(
  pretrained=False,
  **kwargs
  ):
  model = MyModel()
  if pretrained:
     ptw = 'https://url.com/w.pth'
     model.load_state_dict(
      torch.hub.load_state_dict_from_url(ptw)
    )
  return model
```

```
repo = ...
model = torch.hub.load(
  repo,
  my_model,
  pretrained=True
)
```

PyTorch: Freeze Model Parameters

```python
# Do not compute gradients in backward pass
for param in model_conv.parameters():
  param.requires_grad = False
```

PyTorch: Overwrite Pre-Trained Layers

```
model = nn.Sequential(
  nn.Linear(784, 256),
  nn.ReLU(),
  nn.Linear(256, 64),
  nn.ReLU(),
  nn.Linear(64, 10)
)

print(model)
# Sequential(
#   (0): Linear(...)
#   (1): ReLU()
#   (2): Linear(...)
#   (3): ReLU()
#   (4): Linear(...)
# )
```

```
for param in model.parameters()[:-1]:
  param.requires_grad = False

n_in_features = model[-1].in_features

# Swap last linear layer
# with another (untrained) one
model[-1] = nn.Linear(n_in_features, 5)
```

Hyperparameter Tuning

Hyper-parameters can have a huge impact on the model, and the hyperparameter space is large.

There are several libraries for hyperparameter tuning:

- Ray Tune (`https://docs.ray.io`)
- Optuna (`https://optuna.org`)
- Hyperopt (`http://hyperopt.github.io/hyperopt/`)
- ...

High-Level Libraries for PyTorch

PyTorch is rather bare-bones. There are many library built on top of it which require to write much less boilerplate code (training loop, builtin metrics, learning rate scheduling, ...):

- PyTorch Ignite
- FastAI
- Keras 3.0 (PyTorch, TensorFlow, JAX)
- ...

PyTorch Ignite Example

```python
from ignite.engine import create_supervised_trainer
...
trainer = create_supervised_trainer(model, optimizer, loss_fn, device)
trainer.run(tran_loader, max_epochs=5)
```

PyTorch Ignite Example

```
from ignite.engine import Engine
...
def train_step(engine, batch):
    model.train()
    optimizer.zero_grad()
    x, y = batch[0].to(device), batch[1].to(device)
    y_pred = model(x)
    loss = criterion(y_pred, y)
    loss.backward()
    optimizer.step()
    return loss.item()

trainer = Engine(train_step)
trainer.run(tran_loader, max_epochs=5)
```

Keras 3.0 Example

```
model = keras.Sequential([
  keras.Input(shape=input_shape),
  layers.Conv2D(32,
    kernel_size=(3, 3),
    activation="relu"
  ),
  layers.MaxPooling2D(
    pool_size=(2, 2)
  ),
  ...
  layers.Flatten(),
  layers.Dense(
    num_classes,
    activation="softmax"
  )])
```

```
model.compile(
  loss="categorical_crossentropy",
  optimizer="adam",
  metrics=["accuracy"]
)

model.fit(
  x_train, y_train,
  batch_size=batch_size,
  epochs=epochs,
  validation_split=0.1
)

score = model.evaluate(
  x_test, y_test, verbose=0
)
```

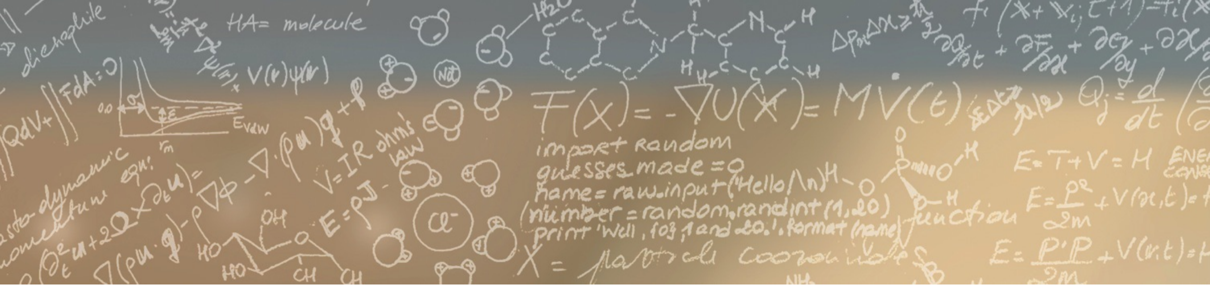
Exercises

Regularization and data augmentation:

- Train a CNN with and without dropout layers
- Train a CNN with and without data augmentation
- Save and load model weights (early stopping)

Transfer learning:

- Modify VGG-19 to work with only 5 classes
- Freeze retained VGG-19 parameters
- Apply transfer learning to the new data



Thank you for your attention!

Why the Validation Loss is Lower than the Traning Loss?

- Regularization is applied during training but not inference
- Training loss is computed during each epoch, validation loss after each epoch
  - Shift loss of $1/2$ epoch
- Validation set might be easier than the training set
- Training set leaked into the validation set