Additional Techniques for Training Neural Networks

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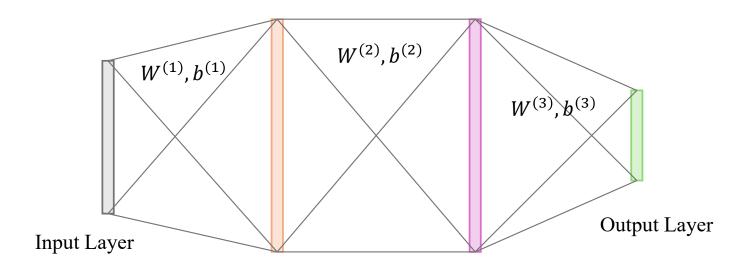
Section-1: Regularization

Imagine a Neural Network (MLP) with 50 input features and 10 class labels. Suppose, we have two hidden layers each with size = 100 (i.e. 100 hidden nodes in each hidden layers). How many parameters does this NN have?

 $W^{(1)}$: weight of the first linear layer; $b^{(1)}$: bias of the first linear layer

 $W^{(2)}$: weight of the second linear layer; $b^{(2)}$: bias of the second linear layer

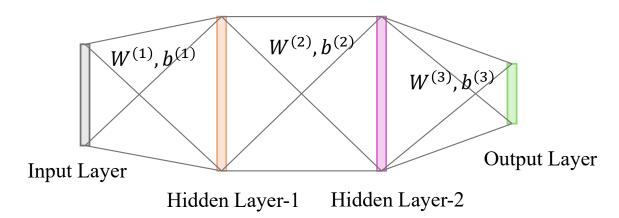
 $W^{(3)}$: weight of the third linear layer; $b^{(3)}$: bias of the third linear layer



Hidden Layer-1

Hidden Layer-2

Imagine a Neural Network (MLP) with 50 input features and 10 class labels. Suppose, we have two hidden layers each with size = 100 (i.e. 100 hidden nodes in each hidden layers). How many parameters does this NN have?



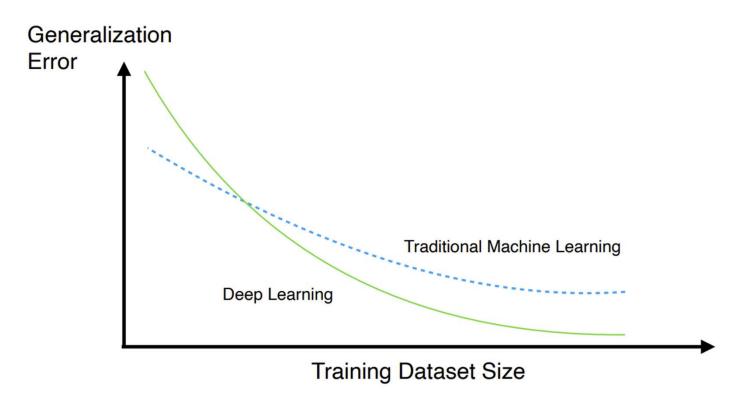
Size of $W^{(1)}=size$ of first hidden layer \times input $size=50\times100=5{,}000$; Size of $b^{(1)}=size$ of first hidden layer =100

Size of $W^{(2)}=size$ of second hidden layer \times size of first hidden layer $=100\times100=10,000$; Size of $b^{(2)}=size$ of second hidden layer =100

Size of $W^{(3)}=size$ of output layer \times size of second hidden layer $=10\times100=1000$; Size of $b^{(3)}=size$ of output layer =10

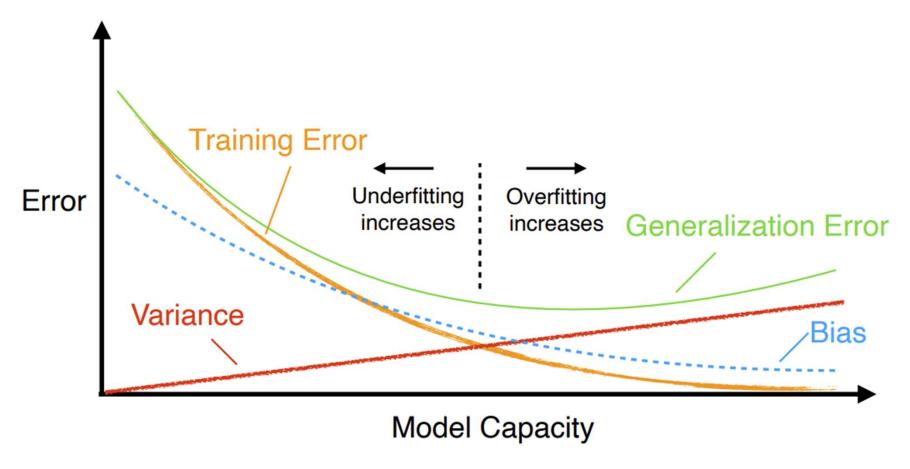
Total number of parameters: (5000+100) + (10000+100) + (1000+10) = 16210

So, our multi-layer neural network contains a lots of parameters. Having a lot of parameter means the model will need huge amount of data to train properly. i.e. why deep learning architectures (i.e. neural nets with multiple layers) works best with huge amount of data.



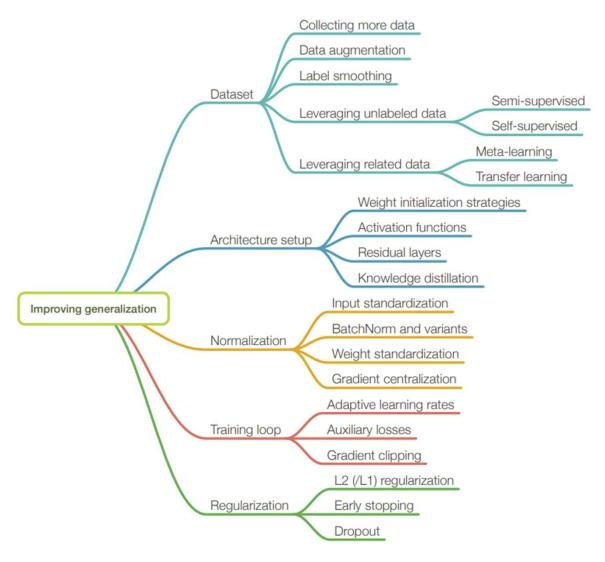
What if we do not have enough training data or the model is too complex?

The old evil: Bias-Variance Trade off



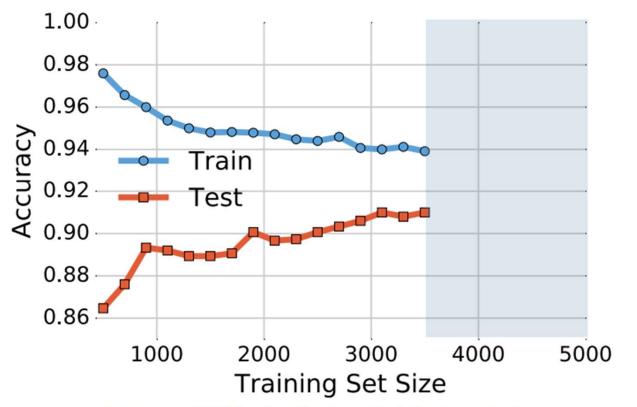
Capacity: abstract concepts ≈ number of model parameters × how efficiently the parameters are used

Improving generalization performance



Avoid overfitting with more data

Often, the best way to reduce overfitting is collecting more data



Softmax on MNIST subset (test set size is kept constant)

However, collecting more data in practice

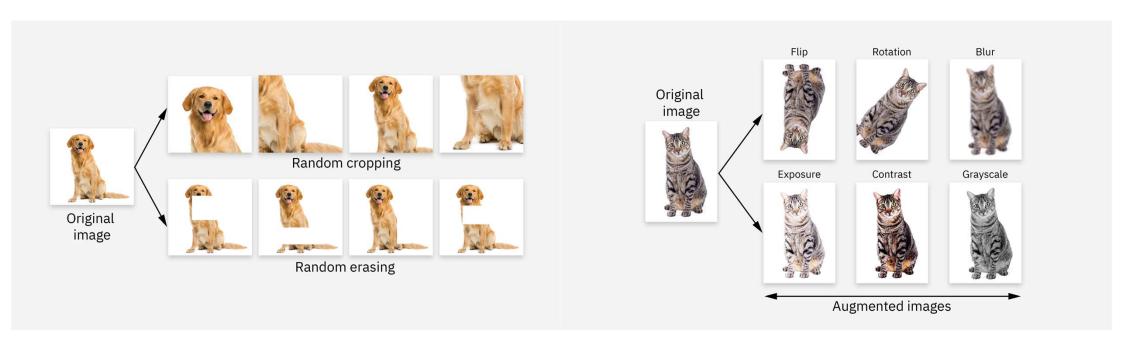
- Requires more time to gather the data.
- More cost involved in gathering the data.
- Can have other constraints.

Hence, researchers and practitioners often tries to come up with strategies to augment the existing dataset.

Data augmentation

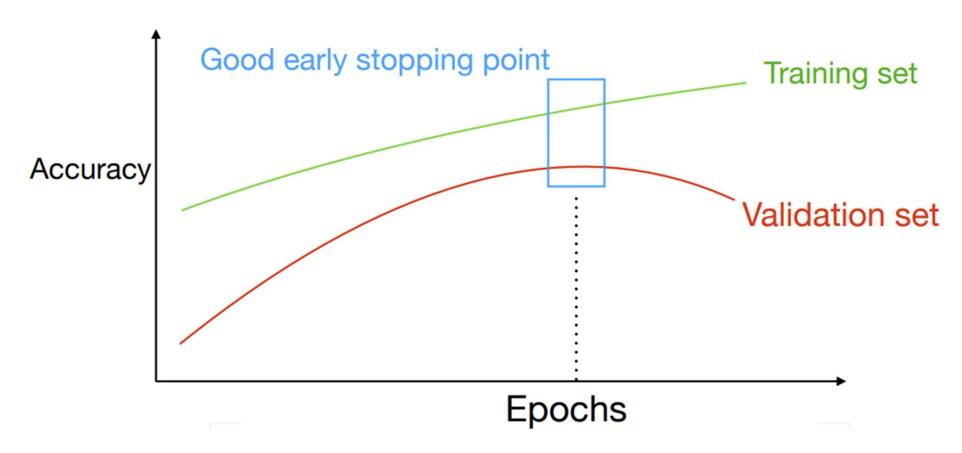
Sometimes, we can enlarge the training dataset by adding little variations of the original dataset. This is called **data** augmentation.

This method is mostly popular in image dataset (computer vision) or sometimes in texts. But for tabular dataset this method doesn't work very well.



Early Stopping

Reduce overfitting by observing the training / validation accuracy gap during training and then stop at the "right" point.



Early stopping is not very common these days.

Early Stopping

35 model.load state dict(torch.load("best model.pt"))

```
1 best_val_loss = float("inf")
                                                                           → Define the early stopping criteria
   patience, counter = 3, 0 # stop if no improvement for 3 epochs
4 for epoch in range(100):
      # ---- Training ----
      model.train()
      for X, y in train_loader:
          optimizer.zero grad()
          loss = criterion(model(X), y)
10
          loss.backward()
11
          optimizer.step()
12
13
      # ---- Validation ----
14
      model.eval()
15
      val loss = 0
16
      with torch.no grad():
17
          for X, y in val_loader:
                                                                            Keep track of validation loss
18
              val loss += criterion(model(X), y).item()
      val loss /= len(val loader)
19
20
21
      print(f"Epoch {epoch+1}, Val Loss: {val loss:.4f}")
22
23
      # ---- Early stopping ----
24
      if val loss < best val loss:
                                                                              If validation loss is less than best validation loss, we will set
25
          best val loss = val loss
                                                                              best_val_loss = val_loss and reset the counter to zero
26
          torch.save(model.state dict(), "best model.pt")
27
          counter = 0
28
      else:
29
          counter += 1
                                                                              If validation loss doesn't improve for 3 epochs, then we
30
          if counter >= patience:
              print("Early stopping triggered!")
31
                                                                              will stop model training.
32
              break
33
34 # Load best model
```

Adding L2 penalties to the loss

$$L_{2} - Regularized \ Cost \ (W, b) = \underbrace{\frac{1}{n} \sum_{i=1}^{n} \mathcal{L}(y^{[i]}, \hat{y}^{[i]})}_{\text{Loss function}} + \underbrace{\frac{\lambda}{n} \sum_{l=1}^{L} \left| \left| W^{(l)} \right| \right|_{F}^{2}}_{\text{L}_{2} \text{ regularization term}}$$

Where, $\left| \left| W^{(l)} \right| \right|_F^2$ is the squared Frobenius Norm of the Weight Matrix of layer $-l = \sum_i \sum_i \left(w_{i,j}^{(l)} \right)^2$

 λ is the regularization parameter.

 L_2 regularization is also called **Thikonov regularization**. It performs "weight shrinkage" or penalty against complexity.

Dropout

Dropout in a Nutshell: dropping nodes

How do we drop nodes practically / efficiently?

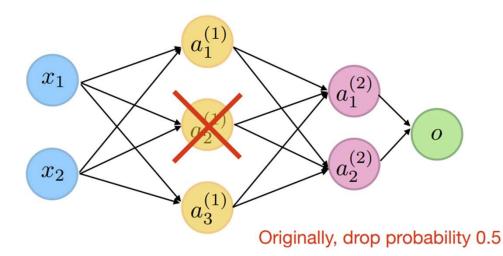
Bernoulli Sampling (during training):

- p := drop probability, usually 0.5 but any value between 0.2 to 0.8 works well in practice.
- v := random sample from uniform distribution in range [0,1]. Where, size of v = size of the nodes in the layer
- $\forall v_i \in v : v_i \leftarrow 0 \text{ if } v_i we will take each values in <math>v$ and if those values are less than p we set it to 0
- Final activation $\tilde{a} = a \odot v$ [\odot denotes element wise product]
- By this $p \times 100\%$ of the activations **a** will be zeroed and rest $(1-p) \times 100\%$ of the activation will be active.
- The surviving activations are scaled by $\frac{1}{1-p}$ to keep the expected value of the activations consistent.

During inference (making predictions):

- No dropout is applied.
- All neurons are active.
- No scaling is needed, since scaling was already handled during training.

Dropout



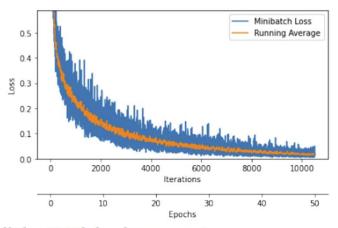
(but 0.2-0.8 also common now)

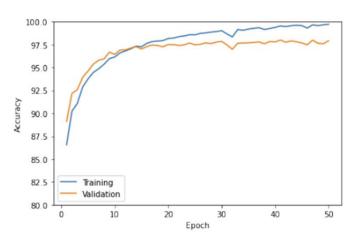
- Dropout reduces overfitting as it prevents the network from relying too heavily on specific neurons or features.
- It acts like an ensemble. Each training step (epoch) samples a different "thinned" subnetwork, and at the inference, you use the average effect of many subnetworks.
- It improves generalization and leads to better performance on unseen/test data.

```
1 import torch
 2 import torch.nn as nn
   class MLP(nn.Module):
       def __init__(self, input_size, hidden_size_1, hidden_size_2,
                    num classes, drop proba):
           super(MLP, self). init ()
10
           self.network = nn.Sequential(
11
               nn.Linear(input_size, hidden_size_1),
12
               nn.ReLU(),
13
               nn.Dropout(drop_proba)
14
               nn.Linear(hidden size 1, hidden size 2),
15
               nn.ReLU(),
               nn.Dropout(drop_proba)
16
17
               nn.Linear(hidden size 2, num classes)
18
19
20
       def forward(self, x):
21
           logits = self.network(x)
22
           return logits
23
24
   for epoch in range(NUM EPOCHS):
25
       model.train()
26
       for batch idx, (features, targets) in enumerate(train loader):
27
           ### codes for training ###
28
29
       model.eval()
30
       with torch.no grad():
31
           ### codes for eval ###
```

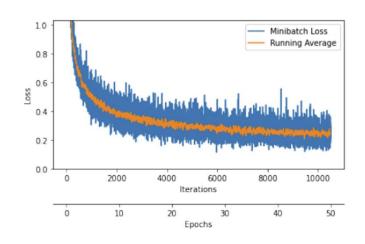
Dropout

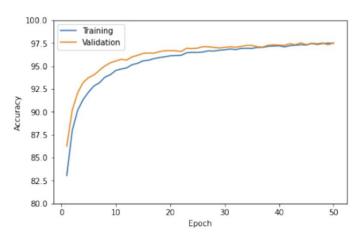
Without dropout:





With 50% dropout:

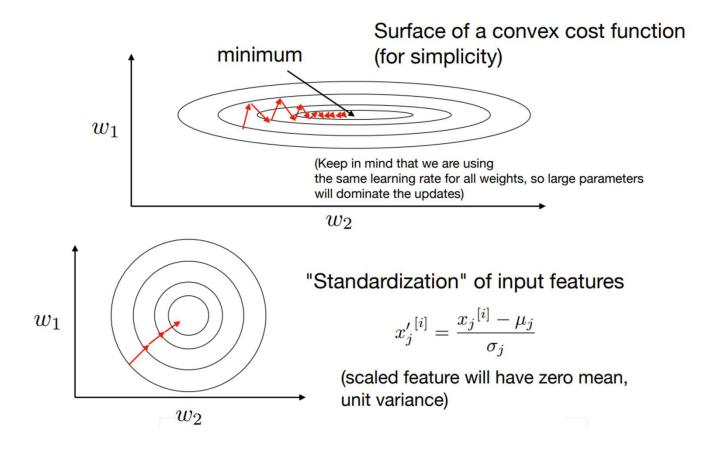




Section-2: Normalization

Feature/Input Normalization

Why do we normalize inputs for Gradient Descent?

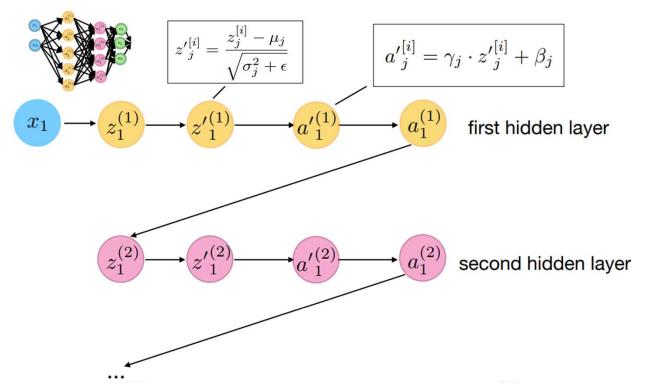


However, normalizing the inputs / features only affects the first hidden layer. What about the other hidden/output layers?

Batch Normalization

Key Concepts

- Normalizes the hidden layer inputs.
- Helps with exploding /vanishing gradient problems.
- Can increase raining stability and convergence rate.
- Can be understood as additional (normalization) layers (with additional parameters).



 γ_j and β_j are the learning parameters

 β_i makes the bias redundant

Hence, we use batchnorm without bias

Batch Normalization with Dropout

```
1 import torch
2 import torch.nn as nn
4 class MLP(nn.Module):
                                                                           Linear → BatchNorm1d → ReLU → Dropout
      def __init__(self, input_size, hidden_size_1, hidden_size_2,
                  num_classes, drop_proba):
          super(MLP, self).__init__()
9
10
          self.network = nn.Sequential(
                                                                             During inference/prediction BatchNorm use
11
              nn.Linear(input_size, hidden_size_1, bias=False),
                                                                              global training set mean and varaince
12
             nn.BatchNorm1d(hidden size 1)
13
             nn.ReLU(),
14
             nn.Dropout(drop_proba)
15
             nn.Linear(hidden size 1, hidden size 2, bias=False),
                                                                             Uses exponentially weighted average (moving
16
              nn.BatchNorm1d(hidden size 1)
17
             nn.ReLU(),
                                                                              average) of mean and variance.
18
             nn.Dropout(drop proba)
19
              nn.Linear(hidden size 2, num classes)
20
21
22
      def forward(self, x):
23
          logits = self.network(x)
                                                                   mean = momentum * mean + (1-momentum) * sample mean
24
          return logits
25
  for epoch in range(NUM_EPOCHS):
27
      model.train()
28
      for batch_idx, (features, targets) in enumerate(train_loader):
29
          ### codes for training ###
30
31
      model.eval()
32
      with torch.no grad():
          ### codes for eval ###
```

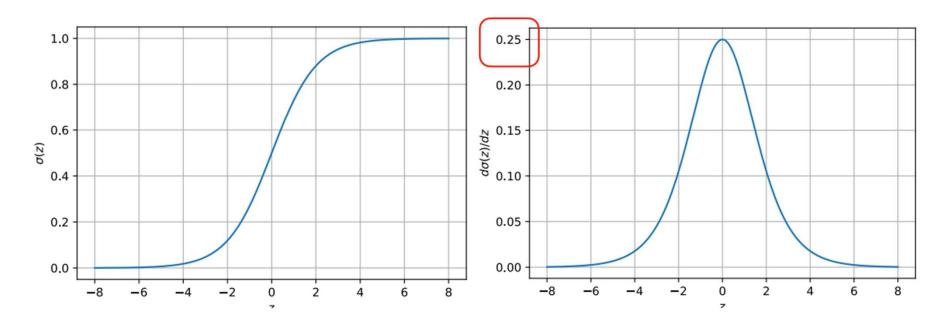
Batch Normalization

```
def train_model(model, num_epochs, train_loader,
               valid_loader, test_loader, optimizer, device):
    start_time = time.time()
    minibatch_loss_list, train_acc_list, valid_acc_list = [], [], []
    for epoch in range(num_epochs):
       model.train()
       for batch_idx, (features, targets) in enumerate(train_loader):
           features = features.to(device)
           targets = targets.to(device)
           # ## FORWARD AND BACK PROP
           logits = model(features)
           loss = torch.nn.functional.cross_entropy(logits, targets)
           optimizer.zero_grad()
           loss.backward()
                                                                        don't forget model.train()
           # ## UPDATE MODEL PARAMETERS
                                                                        and model.eval()
           optimizer.step()
           # ## LOGGING
                                                                        in training and test loops
           minibatch_loss_list.append(loss.item())
           if not batch_idx % 50:
               print(f'Epoch: {epoch+1:03d}/{num_epochs:03d} '
                     f'| Batch {batch_idx:04d}/{len(train_loader):04d} '
                     f' | Loss: {loss:.4f}')
       model.eval()
       with torch.no_grad(): # save memory during inference
           train_acc = compute_accuracy(model, train_loader, device=device)
```

Vanishing and Exploding Gradient Problem

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

$$\frac{d}{dz}\sigma(z) = \frac{e^{-z}}{(1+e^{-z})^2} = \sigma(z)(1-\sigma(z))$$



Assume, we have the largest gradient:

$$\frac{d}{dz}\sigma(0.0) = \sigma(0.0)(1 - \sigma(0.0)) = 0.25$$

Even then, for, e.g., 10 layers, we degrade the other gradients substantially!

$$0.25^{10} \approx 10^{-6}$$

Section-3: Weight initialization

Why weight initialization matters?

- Neural networks learn by adjusting weights.
- Poor initialization can cause:
 - Vanishing gradients: happens when weights are too small.
 - Exploding gradients: happens when weights are too large.
 - Slow convergence: the weight update happens slowly.
 - Getting stuck in symmetry: if all weight start with the same value, neurons in a layer receive the same input and produces identical outputs. Backprop gives them identical gradient and they keep updating identically and fails to learn the diversity in features.
- Good initialization gives:
 - Stable gradients: keeps the signal flow stable by avoiding exploding / vanishing gradient problem
 - Faster training and faster convergence.
 - Better accuracy as the neurons in each layer will learn diverse aspects of the features.

Vanishing / Exploding gradient caused by too small or too large weights

Backpropagation repeatedly applies matrix multiplications by weight matrices *and* multiplies by activation derivatives. If the typical scale of those multipliers is <<1, the product decays exponentially with depth \rightarrow vanishing gradients. If the scale is >>1, the product can blow up \rightarrow exploding gradients.

Glorot and He initialization

Glorot (Xavier) initialization [Glorot & Bengio (2010)]

Glorot initialization, also known as **Xavier initialization**, is designed for activation functions that are symmetric around zero, like the **tanh** function or the **sigmoid** function. The method calculates the initial weights from a random distribution with a specific variance.

Uniform Distribution

$$W \sim U \left[-\frac{\sqrt{6}}{\sqrt{n_{in} + n_{out}}}, +\frac{\sqrt{6}}{\sqrt{n_{in} + n_{out}}} \right]$$

Normal Distribution

$$W \sim N\left(0, \sqrt{\frac{2}{n_{in} + n_{out}}}\right)$$

Where n_{in} is the number of input units (fan-in) to the layer and n_{out} is the number of output units (fan-out) from the layer

He initialization [Kaiming He et al. (2015)]

He initialization is a variation of Glorot initialization specifically designed for **ReLU** (**Rectified Linear Unit**) and its variants (like Leaky ReLU). Because ReLU functions are not symmetric and output zero for all negative inputs, they can cause the variance to drop by half at each layer. He initialization accounts for this by adjusting the variance of the initial weights.

Uniform Distribution

$$W \sim U \left[-\frac{\sqrt{6}}{\sqrt{n_{in}}}, +\frac{\sqrt{6}}{\sqrt{n_{in}}} \right]$$

Normal Distribution

$$W \sim N\left(0, \sqrt{\frac{2}{n_{in}}}\right)$$

Weight initialization in PyTorch

PyTorch by default initializes weights by a variation of **Kaiming Uniform** (He initialization)

$$W \sim U\left[-\sqrt{\frac{1}{n_{in}}}, +\sqrt{\frac{1}{n_{in}}}\right]$$
 and biases are initilizaed to $\mathbf{0}$ if bias = True

PyTorch uses a different version of Kaiming Uniform initialization because this initialization method generalizes well for different layers (like linear, conv2d etc.) and different activation functions. However, one can change the default initialization by using **torch.nn.init** module.

```
1 import torch
 2 import torch.nn as nn
 4 class MLP(torch.nn.Module):
       def init (self, num features, num hidden, num classes):
           super(). init ()
           ### 1st hidden layer
10
           self.linear 1 = torch.nn.Linear(num features, num hidden)
11
           nn.init.kaiming_uniform_(self.linear_1.weight, mode='fan_in', nonlinearity='relu') # initializing the weights
12
           nn.init.zeros (self.linear 1.bias)
                                                                     # initializing the bias
13
14
           ### Output Layer
15
           self.linear_out = torch.nn.Linear(num_hidden, num_classes)
16
           nn.init.normal (self.linear out.weight, mean=0.0, std=0.1) # initializing the weights
17
           nn.init.zeros_(self.linear_out.bias)
                                                                        # initializing the bias
18
19
       def forward(self, x):
           ### codes for froward pass ###
```

Section-4: Learning Rate Decay

Learning rate decay

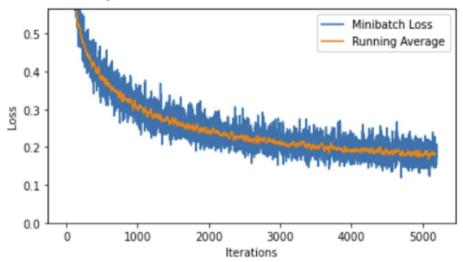
batchsize-1024.

Epoch: 100/100 | Train: 98.45% | Validation: 97.67%

Time elapsed: 4.38 min

Total Training Time: 4.38 min

Test accuracy 97.08%



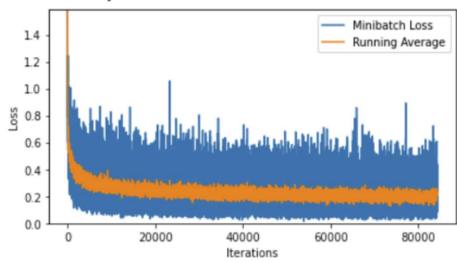
batchsize-64

Epoch: 100/100 | Train: 98.50% | Validation: 97.65%

Time elapsed: 5.59 min

Total Training Time: 5.59 min

Test accuracy 97.18%



- Batch effects: minibatches are samples of training set, hence minibatch loss and gradients are approximations.
- Hence, we usually get oscillations.
- To dampen the oscillations towards the end of the training, we can decay the learning rate.

Learning rate decay

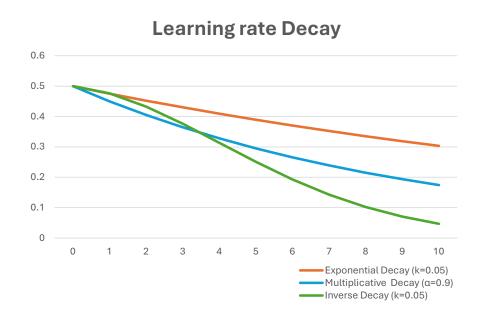
Most common variants of learning rate decay

- 1. Exponential Decay: $\eta_t := \eta_0 \cdot e^{-kt}$; where k is the decay rate.
- 2. Multiplying the decay with some positive fraction: $\eta_t := \alpha \cdot \eta_{t-1}$; where $0 < \alpha < 1$.
- 3. Inverse decay: $\eta_t := \frac{\eta_0}{1+k \cdot t}$; where k is the decay parameter.

And there are many more...

Caveats of using learning rate decay

- Decay can happen too early if the decay parameter is not tuned properly.
- Practical tip: try to train the model without learning rate decay first, then add it later.
- You can also use validation performance (e.g. validation accuracy) to judge whether LR-decay is useful.



Learning rate schedulers in PyTorch

Option-1: Call your own function at the end of each epoch

Option-2: Use one of the built in tools in **torch.optim.lr_scheduler** module

```
for epoch in range(5):
    model.train()
    for batch_idx, (features, targets) in enumerate(train_loader):
        features = features.view(-1, 28*28).to(DEVICE)
        targets = targets.to(DEVICE)
        logits, probas = model(features)
        cost = F.cross_entropy(logits, targets)
        optimizer.zero_grad()
        cost.backward()
        optimizer.step() # UPDATE MODEL PARAMETERS

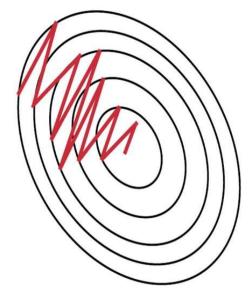
# UPDATE LEARNING RATE
scheduler.step() # don't have to do it every epoch!
```

Section-5: Momentum and Adaptive Learning Rates

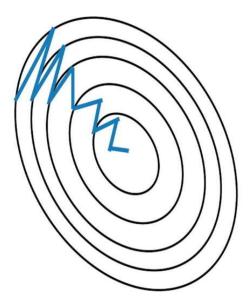
Training with momentum

Key Concept: In momentum learning, we try to accelerate convergence by dampening oscillations using "velocity" (the speed of the "movement" from previous updates)

Momentum helps with dampening oscillations.

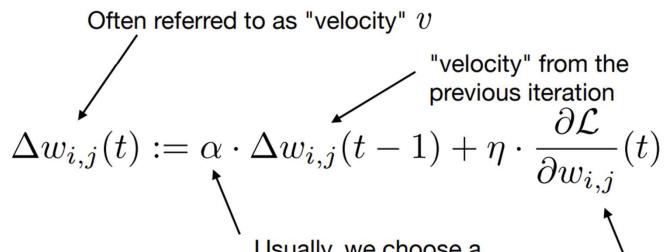


Stochastic Gradient
Descent withhout
Momentum



Stochastic Gradient
Descent with
Momentum

Training with momentum



Usually, we choose a momentum rate between 0.9 and 0.999; you can think of it as a "friction" or "dampening" parameter

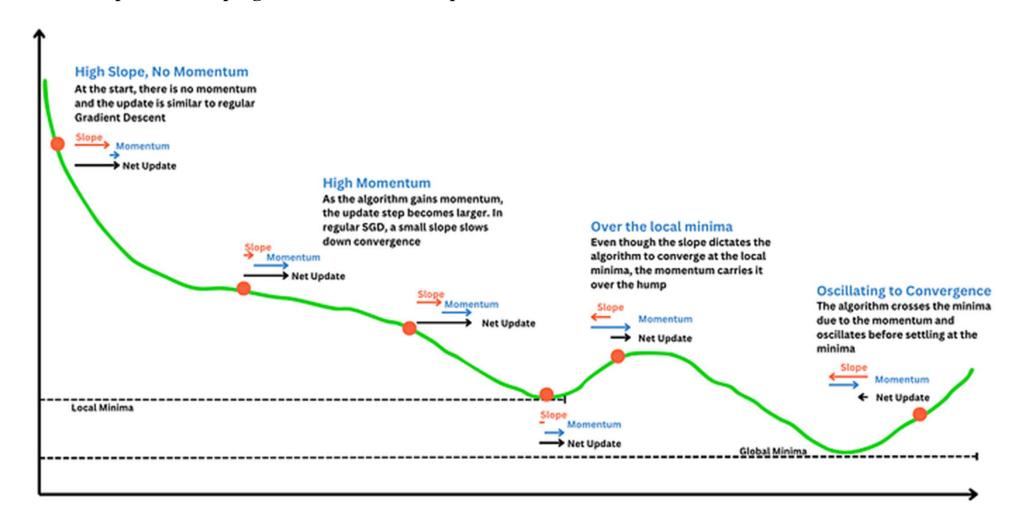
Regular partial derivative/ gradient multiplied by learning rate at current time step t

Weight update using the velocity vector:

$$w_{i,j}(t+1) := w_{i,j}(t) - \Delta w_{i,j}(t)$$

Training with momentum

Momentum helps with escaping the local minima traps



Nesterov's Accelerated Gradient

Nesterov's Accelerated Gradient (NAG), also known as Nesterov's momentum, is a variation of the standard momentum method. It's a "look-ahead" technique that often leads to faster and more stable convergence.

The key difference is that instead of calculating the gradient at the current position, NAG computes the gradient at a point where the parameters *will be* after applying the current velocity. This allows the optimizer to "see ahead" and make a more informed correction.

Normal momentum equation:

Nesterov's momentum (NAG) equation:

$$v_t = \alpha \ v_{t-1} + \eta \ \nabla_w \mathcal{L}(w_t)$$

$$v_t = \alpha \ v_{t-1} + \eta \ \nabla_w \mathcal{L}(w_t - \alpha \ v_{t-1})$$

$$w_{t+1} = w_t - v_t$$

$$w_{t+1} = w_t - v_t$$

The term $(w_t - \alpha v_{t-1})$ represents the "look-ahead" position. By calculating the gradient at this projected position, NAG can anticipate the change in direction and slow down earlier, which helps to avoid overshooting a minimum.

Momentum and NAG in PyTorch

```
# SGD with normal momentum
torch.optim.SGD(model.parameters(), lr=0.01, momentum=0.99)
# SGD with Nesterov momentum
torch.optim.SGD(model.parameters(), lr=0.01, momentum=0.99, nesterov=True)
```

Adaptive Learning Rates

Key Concepts:

- Decrease learning if the gradient changes its direction.
- Increase learning if the gradient stays constant.

Here are some of the most common adaptive learning rate algorithms:

- AdaGrad (Adaptive Gradient Algorithm): Best for sparse data problems, such as in NLP or recommendation systems.
- RMSprop (Root Mean Square Propagation): Often used in deep neural networks (especially in RNNs)
- ADAM (Adaptive Momentum Estimation): Used in wide range of deep learning tasks.
- NADAM (Nesterov-accelerated Adaptive Moment Estimation): Potentially offers faster convergence on complex models.
- ADAMW (ADAM with Weight Decay): Ideal for training large-scale models like Transformers.
- AdaDelta: Useful when a learning rate is not pre-defined, as it dynamically adjusts the step size.

We will talk about ADAM optimization algorithm in more details. ADAM is very popular and widely used in different times of neural network.

Adaptive Moment Estimation (ADAM)

ADAM Algorithm Initialization

- w_0 : Initial parameter vector
- $m_0 \leftarrow 0$ (Initialize first moment vector)
- $v_0 \leftarrow 0$ (Initialize second moment vector)

ADAM Algorithm Weight Update

- $g_t \leftarrow \nabla_w \mathcal{L}(w_t)$: Get the gradients w.r.t. loss function \mathcal{L} at timestep 't'
- $m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 \beta_1) \cdot g_t : Update \ biased \ first \ moment \ estimate$
- $\widehat{m}_t \leftarrow \frac{m_t}{1-\beta_1^t}$: Compute bias corrected first moment estimate
- $v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 \beta_2) \cdot g_t^2$: Update biased second raw moment estimate
- $\hat{v}_t \leftarrow \frac{v_t}{1-\beta_2^t}$: Compute bias corrected second raw moment estimate
- $w_{t+1} \leftarrow w_t \gamma \cdot \frac{\widehat{m}_t}{(\sqrt{\widehat{v}_t} + \epsilon)}$: Update parameters (where γ is the learning rate)

Good default settings that can be used for most of the cases:

- γ (learning rate): 0.001
- $\beta_1 : 0.9$
- $\beta_2 : 0.999$
- $\epsilon : 10^{-8}$

Adaptive Moment Estimation (ADAM)

Why bias correction is needed in ADAM Algorithm

Since m_0 is initialized to 0, in the first few iterations, m_t will be biased towards zero, especially if β_1 is close to 1. To correct this, the algorithm divides m_t by a term that accounts for the number of steps. The **bias-corrected first moment** (\widehat{m}_t) , is:

$$\widehat{m}_t \leftarrow \frac{m_t}{1 - \beta_1^t}$$

Like the first moment, v_0 is initialized to 0, causing a similar bias. Since β_2 is often very close to 1, this bias can be even more pronounced in the early stages, leading to an artificially small denominator in the final update rule and potentially causing the initial steps to be too large. The **bias-corrected second moment** (\hat{v}_t) , is:

$$\hat{v}_t \leftarrow \frac{v_t}{1 - \beta_2^t}$$

ADAM optimizer in PyTorch

Adam optimizer with deafult settings
torch.optim.Adam(model.parameters(), lr=0.001, betas=(0.9, 0.999), eps=1e-8)

Section-6: Hyperparameters in Neural Network

Hyperparameters in Neural Network

Hyperparameters are user-defined and unlike parameters (weights and biases) they are not learnt by data.

Following are the list of different types of hyperparameters mainly in MLP, though few of them are common to other type of neural network architecture.

The grayed out hyperparameters are usually not tuned during hyperparameter tuning.

Architectural Hyperparameters

- Number of hidden layers
- Number of hidden units in each hidden layers
- Regularization technique (for dropout the dropout probability is a hyperparameter)
- Activation functions in hidden layers (ReLU is often default choice)

Learning based Hyperparameters

- Number of epochs
- Minibatch size
- Learning rates (often scheduler is used)
- Optimization algorithm (often the default parameters of a particular optimization algorithm like ADAM works good in practice)

The hyperparameter optimization can be done in various ways like: Random Search, Grid Search or Bayesian optimization. However, in most of the cases the intuition are used to train the neural network efficiently. For example: if the loss vs epoch curve shows zig-zag or oscillatory pattern then it's a good idea to increase the mini-batch size.

Thank You