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# **FIT3181/5215 Deep Learning**

## Week 05: Practical skills in deep learning

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# Outline

- Setting of a machine learning problem

- General loss versus empirical loss

- Gradient vanishing/exploding and network initialization.

- Overfitting and underfitting

- Recipe for overfitting

- Use regularization term, dropout, batch norm, data augmentation, transfer learning
- Label smoothing, data mix-up, cut-mix

- Further reading recommendation

- [Deep Learning, Sections 4.1-4.3, 8.1 -8.5, 11.3, 11.4].
- [Dive into Deep Learning, Chapters 5 and 11].



# Machine learning setting

Not in assessment

## Data-label generative process

$$(x', y') \sim p_{data}(x, y) = p_{data}(x)p_{data}(y | x)$$

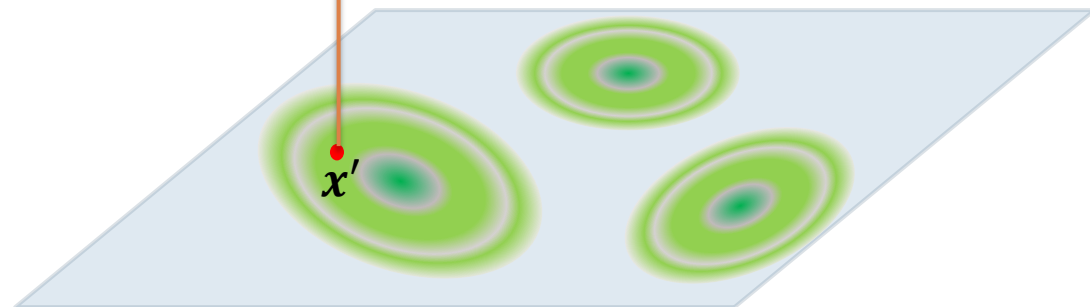
$y' = \mathbf{1 \text{ or } cat}$

$$y' \sim p_{data}(y | x')$$

| Cat<br>(1) | Dog<br>(2) | Lion<br>(3) | Panda<br>(4) |
|------------|------------|-------------|--------------|
| 0.7        | 0.2        | 0.05        | 0.05         |

$p_{data}(y | x')$

Ground-truth labelling mechanism



Data  
space  $\mathcal{X}$

$$x' \sim p_{data}(x)$$

Data distribution

## Dataset collecting process

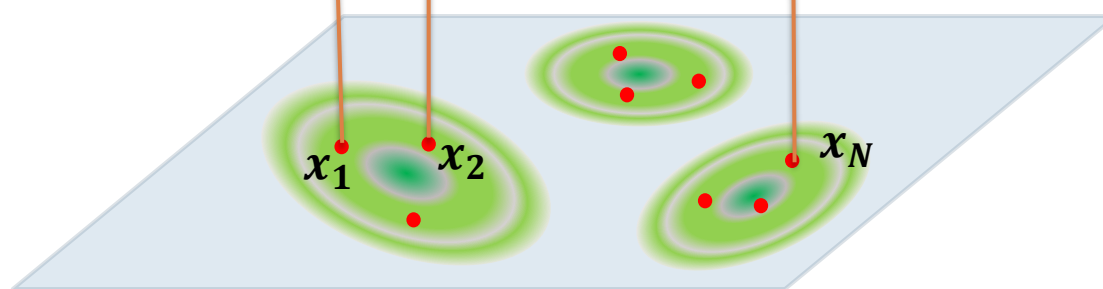
$$D = \{(x_1, y_1), \dots, (x_N, y_N)\}$$

$$(x_i, y_i) \sim p_{data}(x, y) \xleftarrow{N \rightarrow \infty} \tilde{p}_{data}(x, y) = \frac{1}{N} \sum_{i=1}^N \delta_{(x_i, y_i)}(x, y)$$

$$y_1 \sim p_{data}(y | x_1)$$

$$y_N \sim p_{data}(y | x_N)$$

$$y_2 \sim p_{data}(y | x_2)$$



Data  
space  $\mathcal{X}$

$$x_1, \dots, x_N \sim p_{data}(x)$$

Data distribution



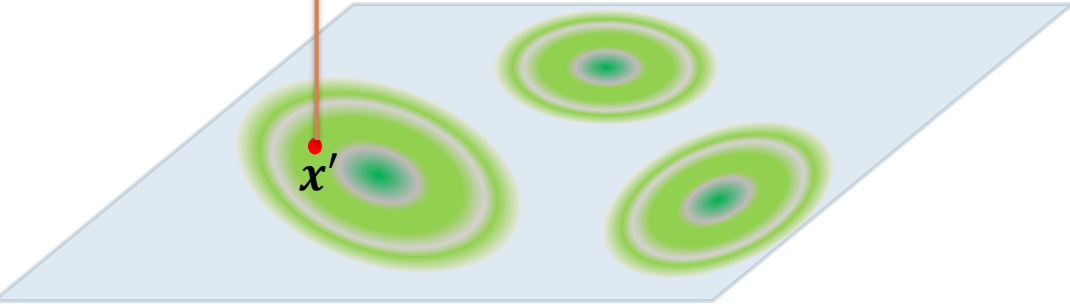
# Machine learning setting

## Data-label generative process

$(x', y') \sim p_{data}(x, y) = p_{data}(x)p_{data}(y | x)$   
 $y' = \mathbf{1 \text{ or } cat}$   
 $y' \sim p_{data}(y | x')$

| Cat<br>(1) | Dog<br>(2) | Lion<br>(3) | Panda<br>(4) |
|------------|------------|-------------|--------------|
| 0.7        | 0.2        | 0.05        | 0.05         |

$p_{data}(y | x')$   
**Ground-truth labelling mechanism**



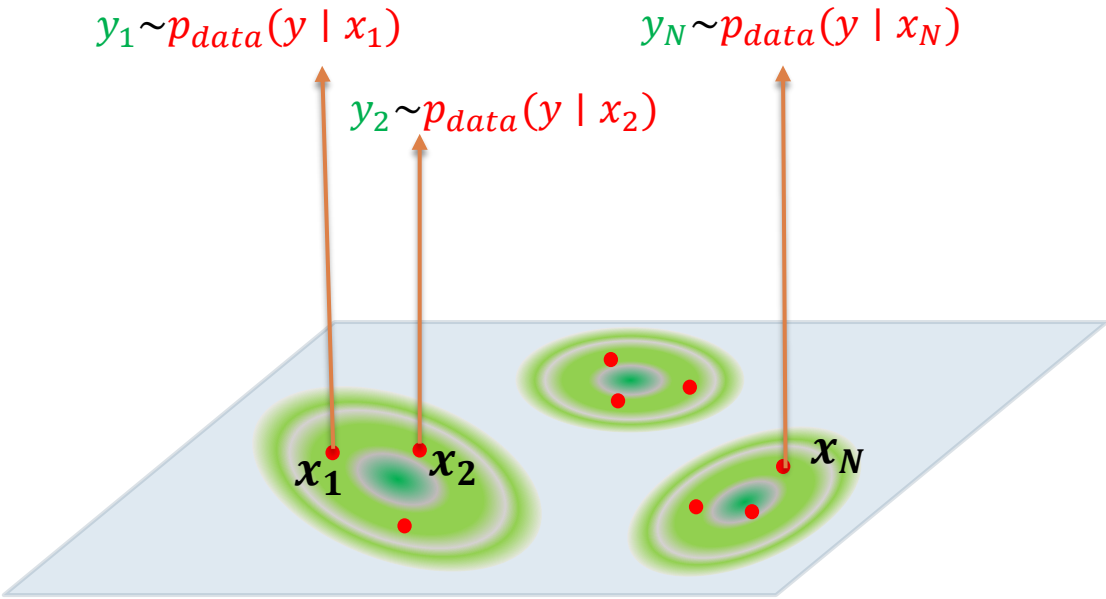
Data space  $\mathcal{X}$   
Data distribution

## Empirical data/label distribution $\tilde{p}_{data}$

| $(x, y)$ | $(x_1, y_1)$ | $(x_2, y_2)$ | ... | $(x_N, y_N)$ |
|----------|--------------|--------------|-----|--------------|
| $p$      | $1/N$        | $1/N$        | ... | $1/N$        |

## Dataset collecting process

$D = \{(x_1, y_1), \dots, (x_N, y_N)\}$   
 $(x_i, y_i) \sim p_{data}(x, y) \xleftarrow{N \rightarrow \infty} \tilde{p}_{data}(x, y) = \frac{1}{N} \sum_{i=1}^N \delta_{(x_i, y_i)}(x, y)$



Data space  $\mathcal{X}$   
Data distribution

Not in assessment



# Machine learning setting

Not in assessment

**Generalization (general) loss**  
(loss on data/label distribution)

$$\mathcal{L}_{gen}(\theta) = \mathbb{E}_{p_{data}} [l(f(x; \theta), y)]$$

**Ideal:**  $\theta^* = \underset{\theta}{\operatorname{argmin}} \mathcal{L}_{gen}(\theta)$

$$(x', y') \sim p_{data}(x, y) = p_{data}(x)p_{data}(y | x)$$

$$y' \sim p_{data}(y | x')$$

$p_{data}(y | x')$

Labelling mechanism

$x' \sim p_{data}(x)$

Data distribution

Data space  $\mathcal{X}$

$N \rightarrow \infty$

Law of large numbers

**Empirical loss**

(loss on a collected training set  $D$ )

$$\mathcal{L}_{emp}(\theta) = \mathbb{E}_{\tilde{p}_{data}} [l(f(x; \theta), y)] = \frac{1}{N} \sum_{i=1}^N l(f(x_i; \theta), y_i)$$

**Reality:**  $\theta^* = \underset{\theta}{\operatorname{argmin}} \mathcal{L}_{emp}(\theta)$

$$D = \{(x_1, y_1), \dots, (x_N, y_N)\}$$

$$(x_i, y_i) \sim p_{data}(x, y) \xleftarrow{N \rightarrow \infty} \tilde{p}_{data}(x, y) = \frac{1}{N} \sum_{i=1}^N \delta_{(x_i, y_i)}(x, y)$$

$$y_1 \sim p_{data}(y | x_1)$$

$$y_2 \sim p_{data}(y | x_2)$$

$$y_N \sim p_{data}(y | x_N)$$

$x_1$

$x_2$

$x_N$

Data space  $\mathcal{X}$

Data distribution

$x \sim p_{data}(x)$

Data distribution



# How Learning Differs from Pure Optimization?

## □ Some important notations:

- $p_{data}(x, y)$ : **existed**, but unknown, distribution of data and label
- $\tilde{p}_{data}(x, y) = \frac{1}{N} \sum_{i=1}^N \delta_{(x_i, y_i)}(x, y)$ : **empirical** data/label distribution - this is what we observed from training data  $\mathbf{D} = \{(x_i, y_i)\}_{i=1}^N$  where  $(x_i, y_i) \stackrel{iid}{\sim} p_{data}(x, y)$ .
- Per-sample loss:  $l(f(x; \theta), y)$

## □ Empirical loss minimisation (pure optimisation):

$$\mathcal{L}_{emp}(\theta) = \mathbb{E}_{\tilde{p}_{data}} [l(f(x; \theta), y)] = \frac{1}{N} \sum_{i=1}^N l(f(x_i; \theta), y_i) \leftarrow \text{Empirical loss (maths)}$$

vs.

## □ But what ML wants is **true generalisation loss**:

Generalisation loss (ML)

$$\mathcal{L}_{gen}(\theta) = \mathbb{E}_{p_{data}} [l(f(x; \theta), y)]$$

How to **achieve this** when we **only have access** to empirical data?



# Optimization Problem in ML and DL

- Most of **optimization problems** in machine learning (deep learning) has the following form:

$$\min_{\theta} J(\theta) = \Omega(\theta) + \frac{1}{N} \sum_{i=1}^N l(y_i, f(x_i; \theta))$$

Regularization term

- $\Omega(\theta) = \lambda \sum_k \sum_{i,j} (w_{i,j}^k)^2 = \lambda \sum_k \|w^k\|_F^2$
- Encourage **simple models**
- Avoid **overfitting**

Empirical loss

- Work well on training set

Guiding principles:

- Occam Razer:** prefer the simplest model that can do well.

How to efficiently solve this optimization problem?  
N is the **training size** and might be very big (e.g.,  $N \approx 10^6$ )

Works well for Deep Learning (non-convex)

## First-order iterative methods

gradient descent, steepest descent  
Use the **gradient** (first derivative)  $g = \nabla_{\theta} J(\theta)$  to update parameters:  
 $w = w - \text{learning rate} \times \text{gradient}$

Works well for convex problems, but not DL


## Second-order iterative methods

Newton and quasi Newton methods  
Use the Hessian matrix (second derivative)  $H = \nabla_{\theta}^2 J(\theta)$  to update parameters



# Optimization Problem in ML and DL

- Most of optimization problems in machine learning (deep learning) has the following form:

$$\min_{\theta} J(\theta) = \Omega(\theta) + \frac{1}{N} \sum_{i=1}^N l(y_i, f(x_i; \theta))$$


What **loss** function should one use?

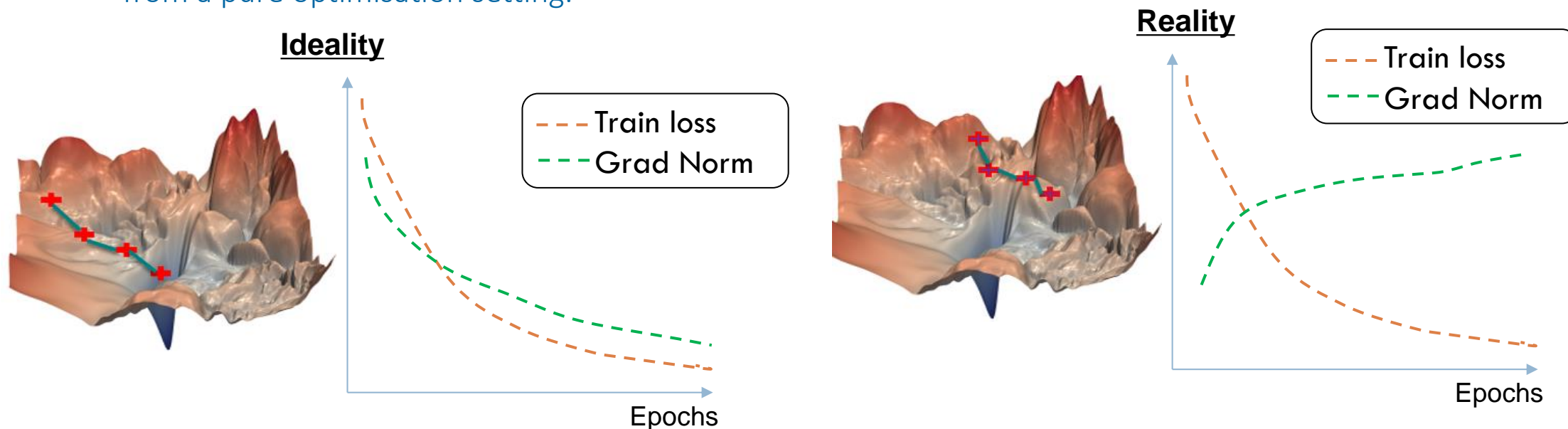
Some typical loss functions used in the classification and regression problems

- 0-1 loss, Hinge loss, Logistic loss (binary classification)
- L1 loss, L2 loss,  $\epsilon$  —insensitive loss (regression)
- Popular surrogate loss: cross-entropy loss (multi-class classification, deep learning)



# How Learning Differs from Pure Optimization?

- Achieving **generalisation capacity** is the holy-grail of machine learning.
  - Empirical risk is prone to **over-fitting**
  - Some times, it is not really feasible if the loss function **does not have useful derivatives** (e.g., 0-1 loss), hence we usually resort to **surrogate loss function**, e.g., cross-entropy, Hinge loss, etc.
- In most cases, DL algorithm **doesn't halt** at **local minimum**
  - It halts when **certain convergence criterion** is **met** (e.g., based on **early stopping** when overfitting start to occur, reach **certain budgets, number of epochs**, etc).
  - For training DL models, it **might stop** when the loss function still has **large derivatives**, which is **different** from a pure optimisation setting.









Challenges in deep learning optimization: gradient  
vanishing, gradient exploding



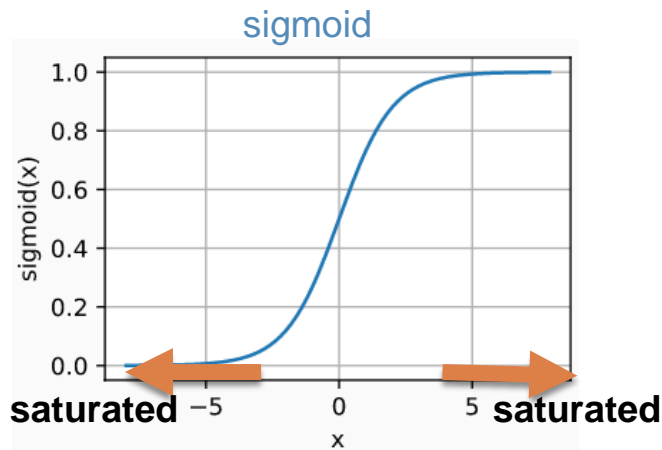
# Gradient vanishing

## Gradient Vanishing

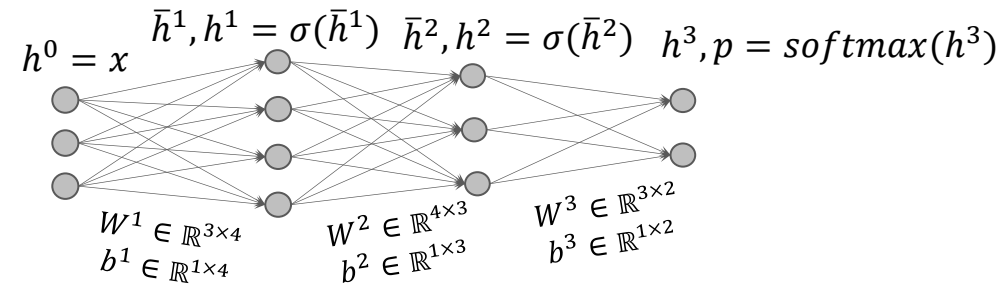
- Gradients get **smaller and smaller** as the algorithm progresses down to the **lower layers**.
  - SGD update leaves the lower layer connection weights **virtually unchanged**, and training **never converges** to a good solution.

## Some activation functions are easy to get saturated

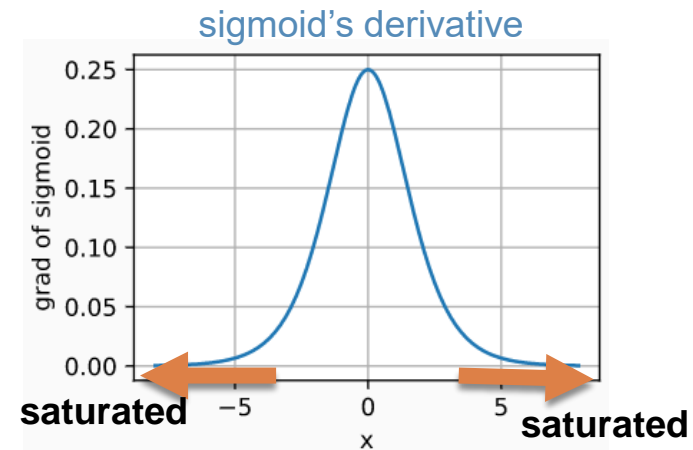
- Sigmoid or tanh



$$\sigma(z) = s(z) = \frac{1}{1 + \exp\{-z\}}$$



$$\begin{aligned} \frac{\partial l}{\partial W^1} &= \frac{\partial l}{\partial h^3} \cdot \frac{\partial h^3}{\partial h^2} \cdot \frac{\partial h^2}{\partial \bar{h}^2} \cdot \frac{\partial \bar{h}^2}{\partial h^1} \cdot \frac{\partial h^1}{\partial \bar{h}^1} \cdot \frac{\partial \bar{h}^1}{\partial W^1} \\ &= \left[ (p^T - 1_y) W^3 \text{diag}(\sigma'(\bar{h}^2)) W^2 \text{diag}(\sigma'(\bar{h}^1)) \right]^T (h^0)^T \end{aligned}$$



$$\sigma'(z) = \sigma(z)(1 - \sigma(z))$$



# Gradient vanishing

## ● Gradient Vanishing

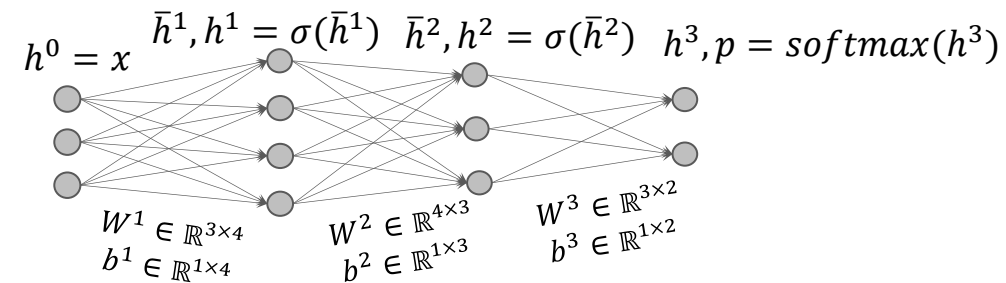
- Gradients get **smaller and smaller** as the algorithm progresses down to the **lower layers**.
  - SGD update leaves the lower layer connection weights **virtually unchanged**, and training **never converges** to a good solution.

## ● Some activation functions are easy to **get saturated**

- Sigmoid or tanh

## ● Recipe

- Activation function plays an important role! Common practice:
  - Avoid sigmoid or saturated activation function
  - ReLU is a common good choice
- Good weight initialization is critical!



$$\begin{aligned} \frac{\partial l}{\partial W^1} &= \frac{\partial l}{\partial h^3} \cdot \frac{\partial h^3}{\partial h^2} \cdot \frac{\partial h^2}{\partial \bar{h}^2} \cdot \frac{\partial \bar{h}^2}{\partial h^1} \cdot \frac{\partial h^1}{\partial \bar{h}^1} \cdot \frac{\partial \bar{h}^1}{\partial W^1} \\ &= \left[ (p^T - 1_y) W^3 \text{diag}(\sigma'(\bar{h}^2)) W^2 \text{diag}(\sigma'(\bar{h}^1)) \right]^T (h^0)^T \end{aligned}$$



# Gradient exploding

## ● Gradient Exploding

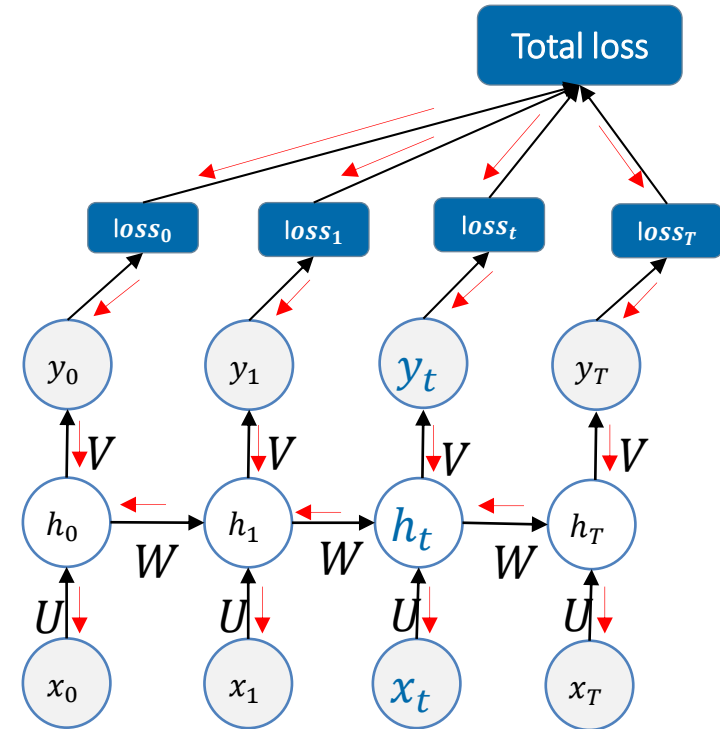
- The gradients can grow **bigger and bigger**, so many layers get **insanely large weight** updates, and the training **diverges**.
- Mostly being encountered in **recurrent neural networks**.

- Often happen for **recursive models** for example **Recurrent Neural Network (RNN)**, **Bidirectional RNN**



### Tip:

- Let simplify  $W$  as **a scalar** in the real-valued set
  - $W^m \rightarrow 0$  if  $|W| < 1$ .
  - $W^m \rightarrow \infty$  if  $|W| > 1$ .



$$\frac{\partial l_T}{\partial h_0} = \frac{\partial l_T}{\partial h_T} \times \underbrace{\frac{\partial h_T}{\partial h_{T-1}} \times \dots \times \frac{\partial h_1}{\partial h_0}}_{\text{Multiplication of many matrices } W}$$

**Multiplication of many matrices  $W$**



# Gradient Clipping

- One way to lessen the **exploding gradients problem** is to simply **clip the gradients** during backpropagation so that they never **exceed** some threshold
  - Either clip by values (direction might change)
  - or clip by norms (keep direction but rescale the magnitude)
- Widely applied to **Recurrent Neural Networks**
- Widely used for NLP tasks, not so much used for CNNs.

```
import torch
import torch.nn as nn
import torch.optim as optim

# Example model
class SimpleModel(nn.Module):
    def __init__(self):
        super(SimpleModel, self).__init__()
        self.fc = nn.Linear(10, 1)

    def forward(self, x):
        return self.fc(x)

# Initialize the model, loss function, and optimizer
model = SimpleModel()
criterion = nn.MSELoss()
optimizer = optim.SGD(model.parameters(), lr=0.01)

# Example training loop
for epoch in range(100):
    optimizer.zero_grad()
    # Example input and target tensors
    inputs = torch.randn(32, 10) # Batch of 32, input size 10
    targets = torch.randn(32, 1) # Batch of 32, target size 1
    # Forward pass
    outputs = model(inputs)
    loss = criterion(outputs, targets)
    # Backward pass
    loss.backward()
    # Gradient clipping by norm
    torch.nn.utils.clip_grad_norm_(model.parameters(), max_norm=2.0)
    # Update model parameters
    optimizer.step()
    # Print loss
    print(f'Epoch {epoch+1}, Loss: {loss.item()}')
```



# Observing Gradient Vanishing and Exploding

## Log the histogram of gradients to TensorBoard

```
def on_epoch_end(self, params):
    epoch = params['epoch']

    # Log scalar values
    if self.log_scalars:
        self.writer.add_scalar('Loss/train', params['train_loss'], epoch)
        self.writer.add_scalar('Loss/validation', params['val_loss'], epoch)
        self.writer.add_scalar('Accuracy/train', params['train_accuracy'], epoch)
        self.writer.add_scalar('Accuracy/validation', params['val_accuracy'], epoch)

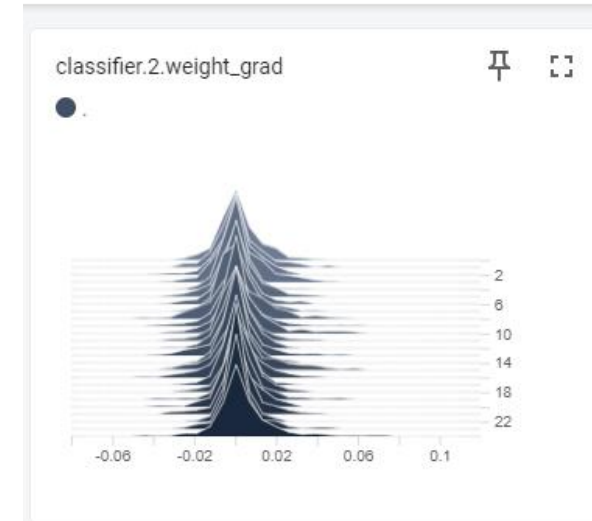
    # Log a batch of images (example with first batch from trainloader)
    if self.log_images:
        dataiter = iter(self.train_loader)
        images, labels = next(dataiter)
        img_grid = vutils.make_grid(images)
        self.writer.add_image('images_batch', img_grid, epoch)

    # Log histogram of model parameters
    if self.log_histograms:
        #log the model parameters
        for name, param in self.model.named_parameters():
            self.writer.add_histogram(name, param, epoch)

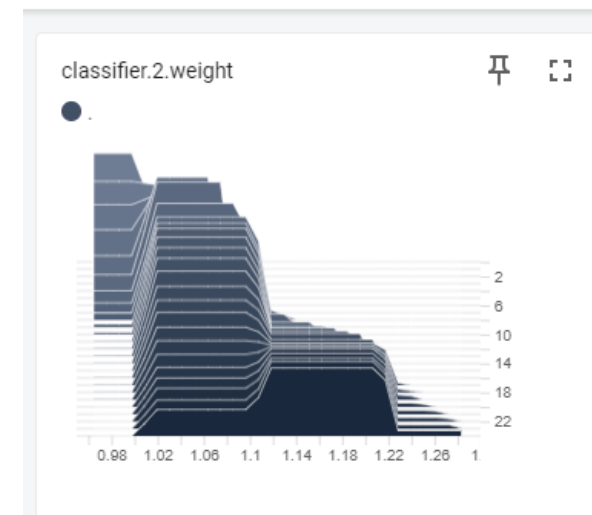
        #log the gradients w.r.t. the model parameters
        num_selected = 100
        subset, _ = torch.utils.data.random_split(val_subset, [num_selected, len(val_subset) - num_selected])
        subset_loader = torch.utils.data.DataLoader(subset, batch_size=num_selected) # Create a dataloader for
        inputs, labels = next(iter(subset_loader)) # Get a batch of data
        inputs, labels = inputs.to(device), labels.to(device) # Move data to device
        outputs = self.model(inputs) # Use self.model instead of models
        loss = self.criterion(outputs, labels)
        loss.backward()
        for name, param in self.model.named_parameters():
            self.writer.add_histogram(name + '_grad', param.grad, epoch)
```

## Using TensorBoard

classifier.2.weight\_grad



classifier.2.weight





## Weight initialization



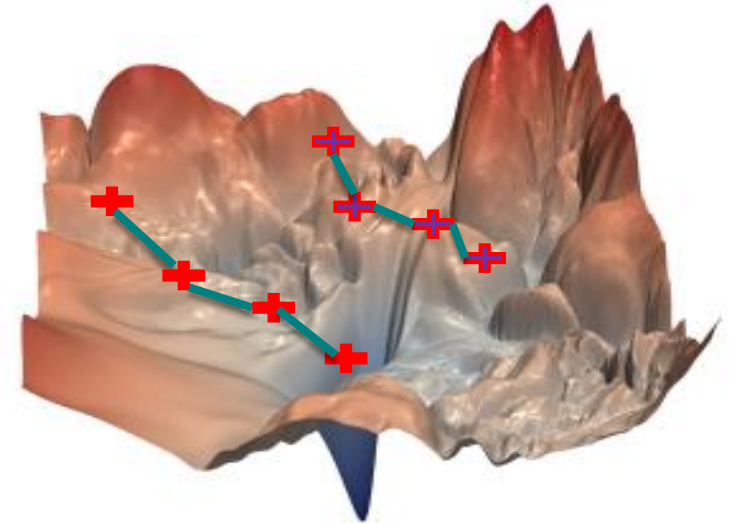
# He and Xavier weight initialization

## ● Initialisation in deep learning training is **crucial**:

- Some optimizers can be **theoretically guaranteed to converge** regardless of initializations
- Deep learning algorithms do not have these luxuries:
  - It is iterative, but optimization deep neural networks is **not yet well understood**
  - **Initial point is extremely important**: it can determine if the algorithm converges, or with some **bad initialisation**, it becomes unstable and fails together

## ● What is a **good weight/filter initialization**?

- **Break the 'symmetry'** of the network: two hidden nodes with the **same input** should have **different weights**.
- The **gradient signal to flow well** in both directions and **don't want** the signal to **die out** or to **explode** and **saturate**.
- **Large initial weights** has **better symmetry breaking** effect, help **avoiding losing signals** and **redundant units**, but could **result in exploding values** during back-ward and forward passes, especially in Recurrent Neural Networks.



**Initialization is important** for training DL models.



# He and Xavier weight initialization

## ● Xavier initialization

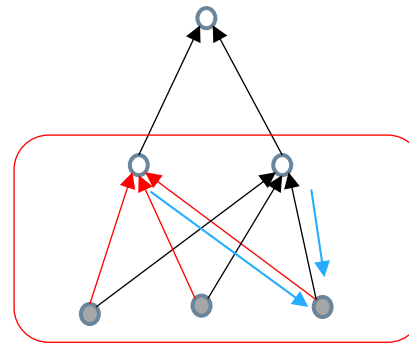
- Try to ensure the **variance of the outputs** of each layer equal to the **variance of its inputs**
- Also need the gradients to have **equal variance** before and **after flowing through a layer** in the **reverse direction**
- Good for **sigmoid** and **tanh** functions
- Not good for ReLU

Gaussian version

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

Uniform alternative

$$w_{Xa} \sim \text{Uniform}\left(-\sqrt{\frac{6}{n_{in} + n_{out}}}, \sqrt{\frac{6}{n_{in} + n_{out}}}\right)$$



$n_{in} = 3$

$n_{out} = 2$

Why  $\sqrt{\frac{2}{n_{in} + n_{out}}}$  ?

---

Understanding the difficulty of training deep feedforward neural networks

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Xavier Glorot

DIRO, Université de Montréal, Montréal, Québec, Canada

Yoshua Bengio

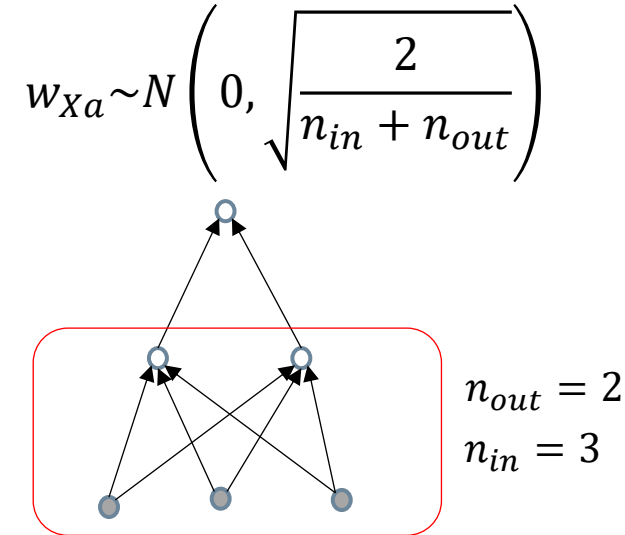
Paper link: <https://proceedings.mlr.press/v9/glorot10a/glorot10a.pdf>



# He and Xavier weight initialization

## □ Xavier initialization

- Ensure the **variance of the outputs** of each layer **equal** to the **variance of its inputs**
- Also need the **gradients** to have **equal variance before** and **after** flowing through a layer in the reverse direction
- Good for **sigmoid** and **tanh** activation functions
- **Not** good for **ReLU**



## □ He initialization

- A **variant of Xavier initialization** where  $\alpha = 1$
- Works better for ReLU.

$$w_{He} \sim N\left(0, \alpha \times \sqrt{\frac{2}{n_{in} + n_{out}}}\right) \quad \alpha = \begin{cases} 1 & \text{if sigmoid} \\ 4 & \text{if tanh} \\ \sqrt{2} & \text{if ReLU} \end{cases}$$



This ICCV paper is the Open Access version, provided by the Computer Vision Foundation.  
Except for this watermark, it is identical to the version available on IEEE Xplore.

**Delving Deep into Rectifiers:  
Surpassing Human-Level Performance on ImageNet Classification**

Kaiming He    Xiangyu Zhang    Shaoqing Ren    Jian Sun  
Microsoft Research

**Paper link:** [https://www.cv-foundation.org/openaccess/content\\_iccv\\_2015/papers/He\\_Delving\\_Deep\\_into\\_ICCV\\_2015\\_paper.pdf](https://www.cv-foundation.org/openaccess/content_iccv_2015/papers/He_Delving_Deep_into_ICCV_2015_paper.pdf)







# Where do we go from here?

- Challenges in deep learning optimisation and how to address them:
  - Local minima, saddle points and complex loss surfaces
  - Gradient vanishing and exploding
  - What we don't cover in this unit (see DL section 8.2):
    - Ill-conditioning problem
    - Long-term dependencies
    - Poor correspondence between local and global structures
    - Theoretical limits of optimisation (but they usually have little use in practice of deep learning)
- Initialization Strategies
- Regularization in deep learning
  - Parameter norm penalty:  $l_1$ ,  $l_2$  regularization
  - Early stopping
  - Dropout
  - Batch normalization
- Choice of optimizers:
  - Basic algorithms: SGD, Momentum, Nesterov Momentum
  - Algorithms with adaptive learning rate: AdaGrad, RMSProp, Adam

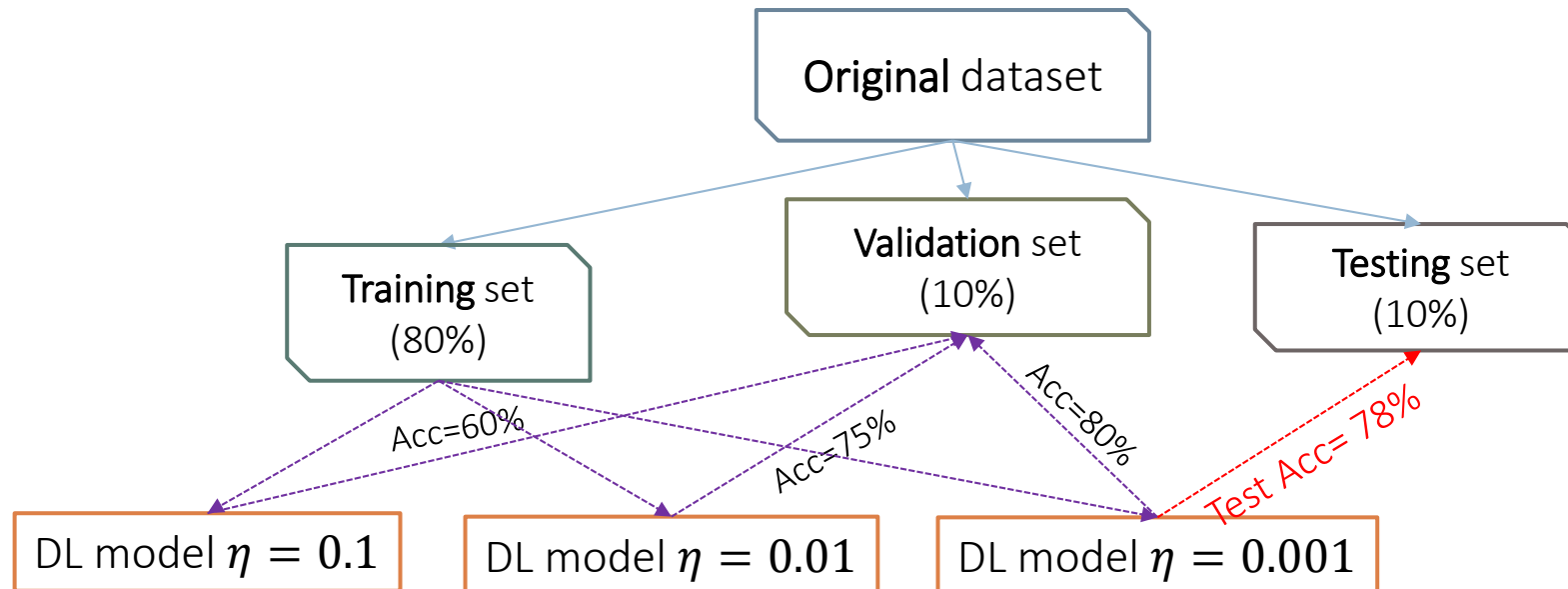


# Overfitting and Regularization in Deep Learning



# Deep Learning Pipeline

- We want to train our DL model on a **training set** such that the **trained model** can predict well **unseen data** in a separate testing set.



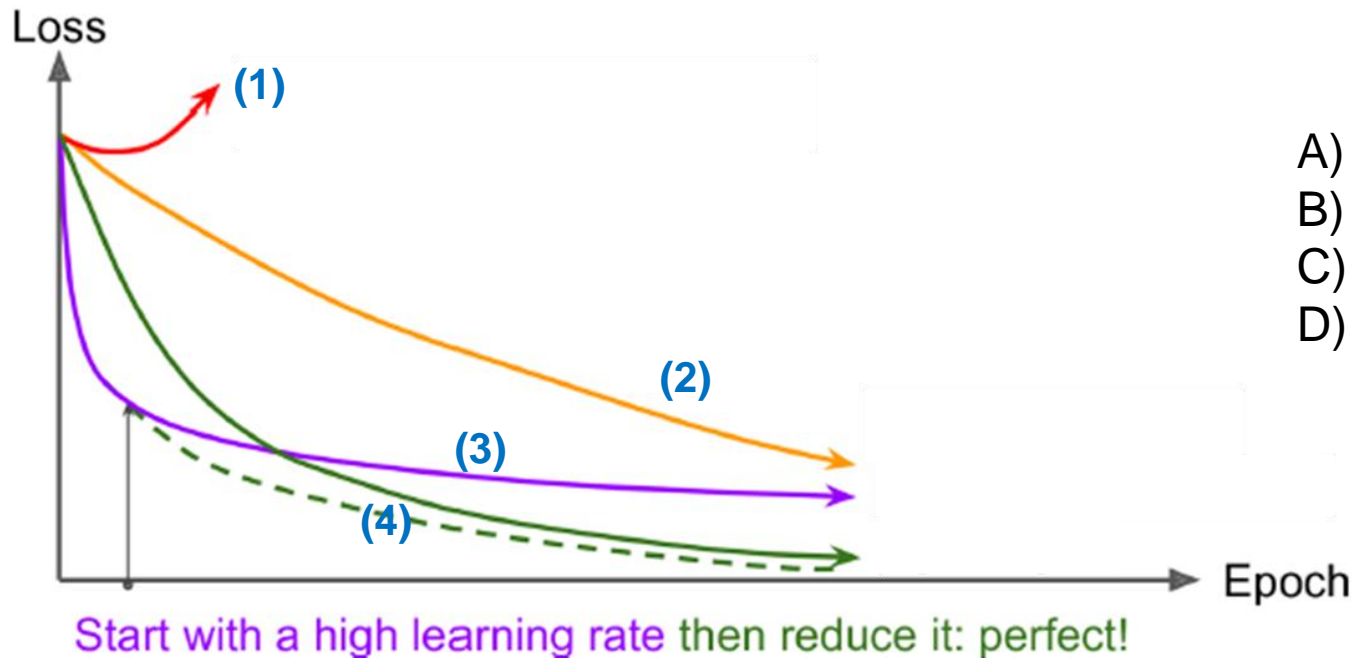
Model parameters: weight matrices, biases, filters which will be learnt

Hyper-parameters to consider: learning rate, #layers, #neurons which need to be tuned



# Deep Learning Pipeline

- We want to train our DL model on a **training set** such that the **trained model** can predict well **unseen data** in a separate testing set.



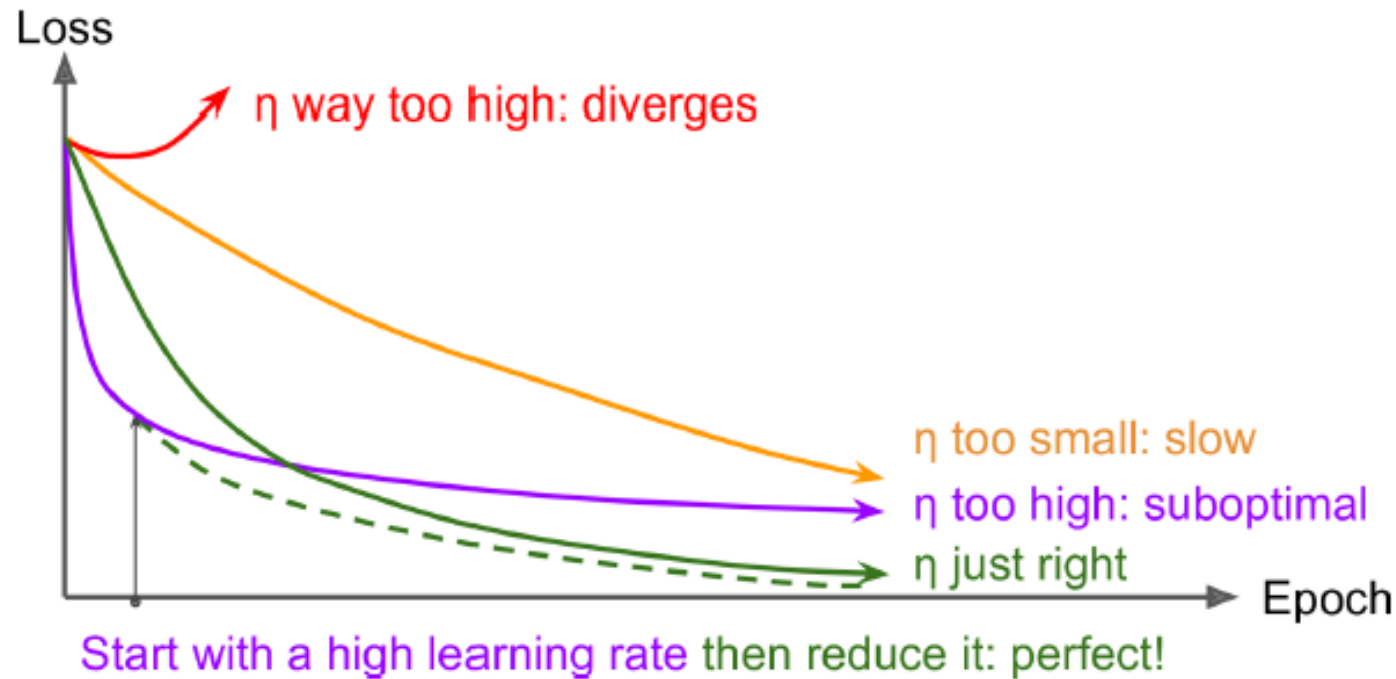
- A) Extremely high
- B) Too high
- C) Too small
- D) Just right

Hyper-parameters to consider: learning rate, #layers, #neurons



# Deep Learning Pipeline

- We want to train our DL model on a **training set** such that the **trained model** can predict well **unseen data** in a separate testing set.



Hyper-parameters to consider: learning rate, #layers, #neurons

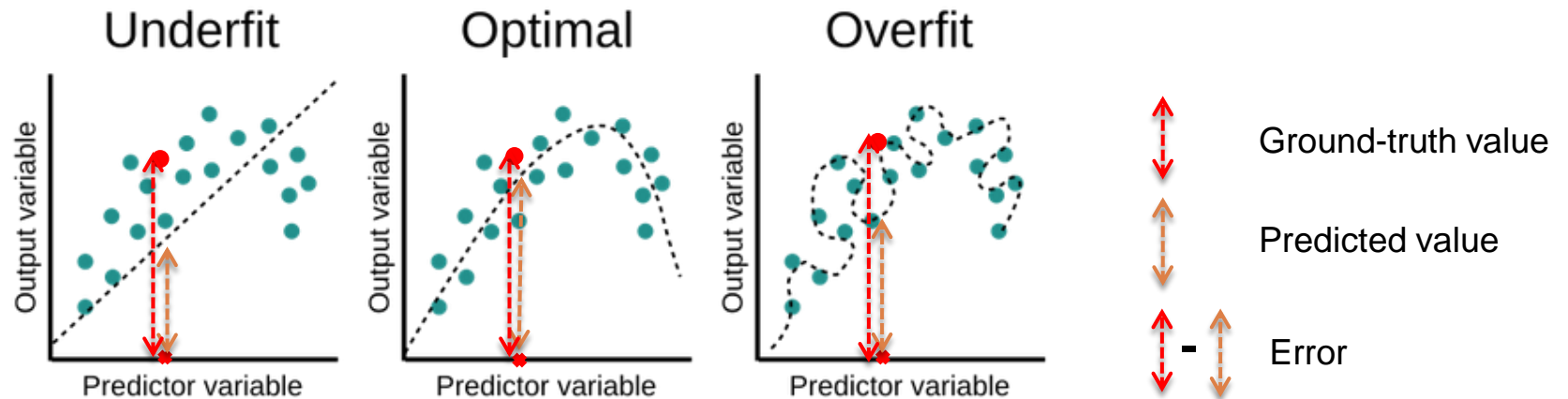


# Regularization and Overfitting

- Three elements in ML and DL
  - **Data**: training data, testing data, validation data
  - **Model**: a **mathematical function**  $f(x; \theta)$  that maps an input instance  $x$  to outcome  $y$
  - **Evaluation**: a **performance metric** to quantitatively measure how well  $f(x; \theta)$  is
- Machine learning as an **optimization process**. **Learning** from data by **optimizing** its loss
  - Define a measure of loss via a **loss function**:  $l(f(x; \theta), y)$
  - Compute its **loss over all training data**  $J(\theta) = N^{-1} \sum_{i=1}^N l(f(x_i, \theta), y_i)$
  - Learning = **finding**  $\theta^*$  that **minimizes** the loss:  $\theta^* = \arg \min_{\theta} J(\theta)$
- What might **go wrong** with this formulation?
  - The choice of **learning function**  $f(x; \theta)$  is too hard to learn
  - The choice of **loss function**  $l(f(x), y)$  is inadequate
  - The model **does well** on training data, but **perform poorly** on unseen test data: **overfitting** problem!



# Overfitting & Underfitting



Overfitting with regression

## Underfitting

- The model is **too simple** to characterise a training set
  - Use linear model to learn from non-linear data

## Overfitting

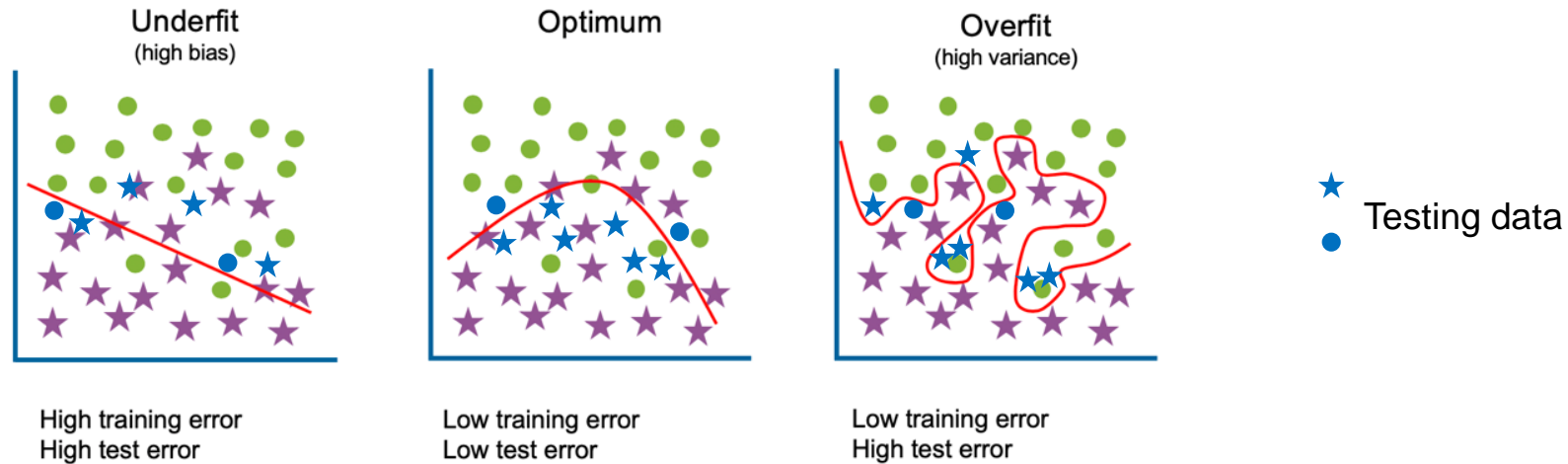
- The model performs **very well** on the **training set**, but **cannot generalise** to perform well on a separate **testing set**
- This is the most common problem in DL since deep networks are very powerful!



# Overfitting in Deep NNs

## Overfitting

**Overfit:** tendency of the network to “memorize” all training samples, leading to poor generalization



**Overfitting with classification**

[Source: <https://www.ibm.com/cloud/learn/overfitting>]

- **Overfitting** occurs when your network models the training data *too well* and fails to generalize to your test (validation) data.
  - Performance measured by errors on “unseen” data.
  - **Minimize error alone on training data is not enough**
  - **Causes: too many layers, too many hidden nodes, and overtrained.**



| Hyperparameter           | Increases capacity when... | Reason   | Caveats   |
|--------------------------|----------------------------|--|---|
| Number of hidden units   | increased                  | Increasing the number of hidden units increases the representational capacity of the model.  | Increasing the number of hidden units increases both the time and memory cost of essentially every operation on the model.  |
| Learning rate            | tuned optimally            | An improper learning rate, whether too high or too low, results in a model with low effective capacity due to optimization failure |   |
| Convolution kernel width | increased                  | Increasing the kernel width increases the number of parameters in the model  | A wider kernel results in a narrower output dimension, reducing model capacity unless you use implicit zero padding to reduce this effect. Wider kernels require more memory for parameter storage and increase runtime, but a narrower output reduces memory cost. |
| Implicit zero padding    | increased                  | Adding implicit zeros before convolution keeps the representation size large   | Increased time and memory cost of most operations.  |
| Weight decay coefficient | decreased                  | Decreasing the weight decay coefficient frees the model parameters to become larger  |   |
| Dropout rate             | decreased                  | Dropping units less often gives the units more opportunities to “conspire” with each other to fit the training set                 |   |

We can also experiment with model capacity itself in parallel.

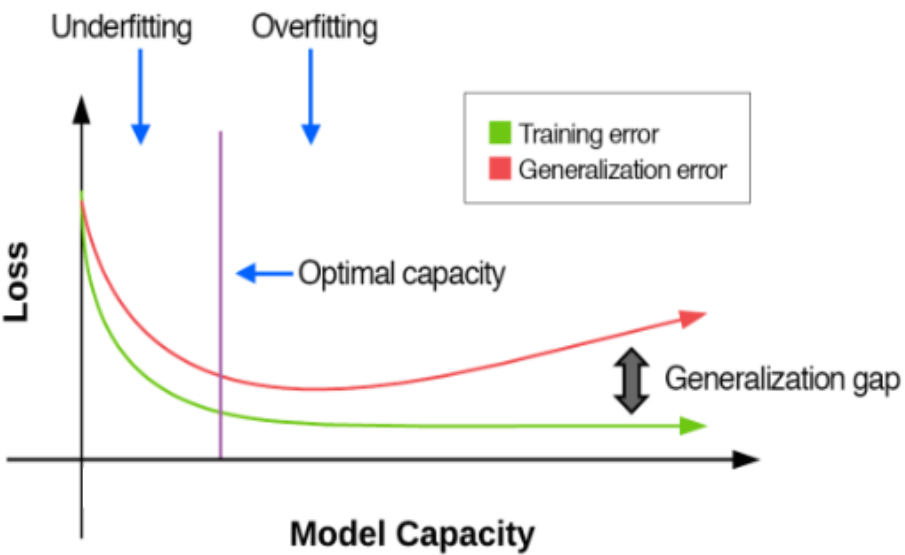


Table 11.1: The effect of various hyperparameters on model capacity.



# Recipe for Overfitting

## ❑ **Early stopping**

- ❑ Stopping the training on time before it becomes overtrained and overly complex.

## ❑ **Train with more data**

- ❑ Expanding the training set to include more data

## ❑ **Data augmentation**

- ❑ Creating many variations of clean data to make the model to generalize better to unseen examples.

## ❑ **Regularization**

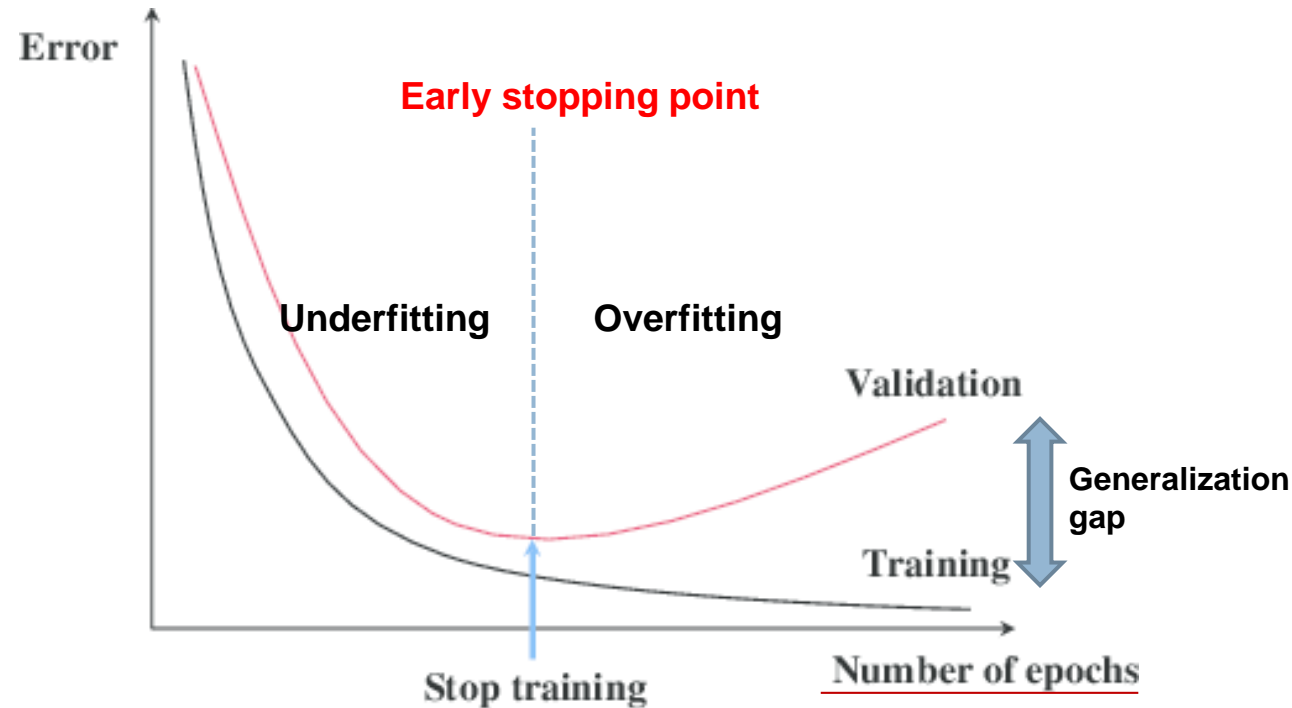
- ❑ Overfitting occurs when a model is too complex comparing with data.
- ❑ Using regularization terms (L1, L2), batch norm, dropout, data mix-up, label smoothing, VAT (virtual adversarial training).

## ❑ **Ensemble methods (not cover in this lecture)**

- ❑ Ensemble learning methods are made up of a set of classifiers and their predictions are aggregated to identify the most popular result.
- ❑ The most well-known ensemble methods are **bagging** and **boosting**.



# Early stopping



- At first, the train and valid losses **gradually drop**, but the model is **not good enough** to characterise data
  - **Underfitting** is happening
- At a certain point, the train loss **still decreases**, while the valid loss **starts increasing**
  - **Overfitting** starts happening and we need to do **early stopping** at this point



# Add Regularization

## Reduce Overfitting

### □ Optimization problem

$$\min_{\theta} J(\theta) = \Omega(\theta) + \frac{1}{N} \sum_{i=1}^N l(y_i, f(x_i; \theta))$$

### □ L2 regularization

$$\Omega(\theta) = \lambda \sum_k \sum_{i,j} (W_{i,j}^k)^2 = \lambda \sum_k \|\mathbf{W}^k\|_F^2$$

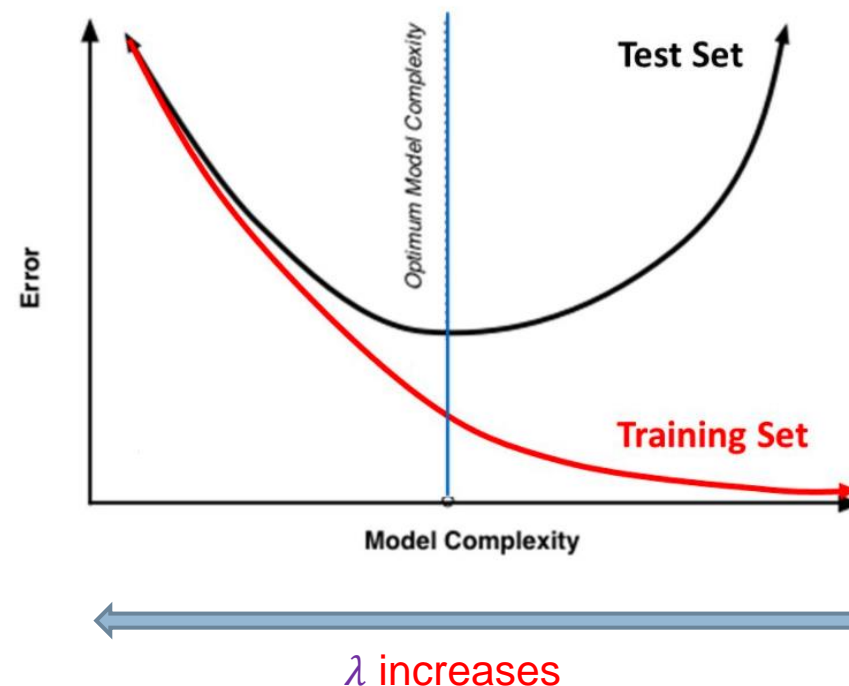
- $\lambda > 0$  is regularization parameter
- Gradient:  $\nabla_{\mathbf{W}^k} \Omega(\theta) = 2\mathbf{W}^k$
- Apply on weights ( $\mathbf{W}$ ) only, not on biases ( $\mathbf{b}$ )

### □ L1 regularization

$$\Omega(\theta) = \lambda \sum_k \sum_{i,j} |W_{i,j}^k|$$

- $\lambda > 0$  is regularization parameter
- Optimization is now much harder – subgradient.
- Apply on weights ( $\mathbf{W}$ ) only, not on biases ( $\mathbf{b}$ )

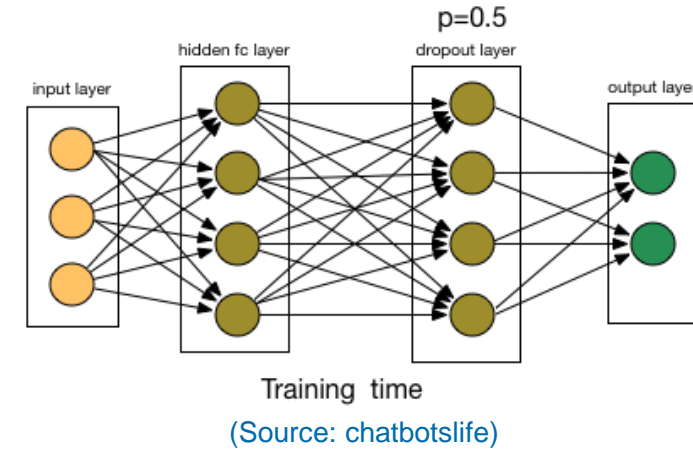
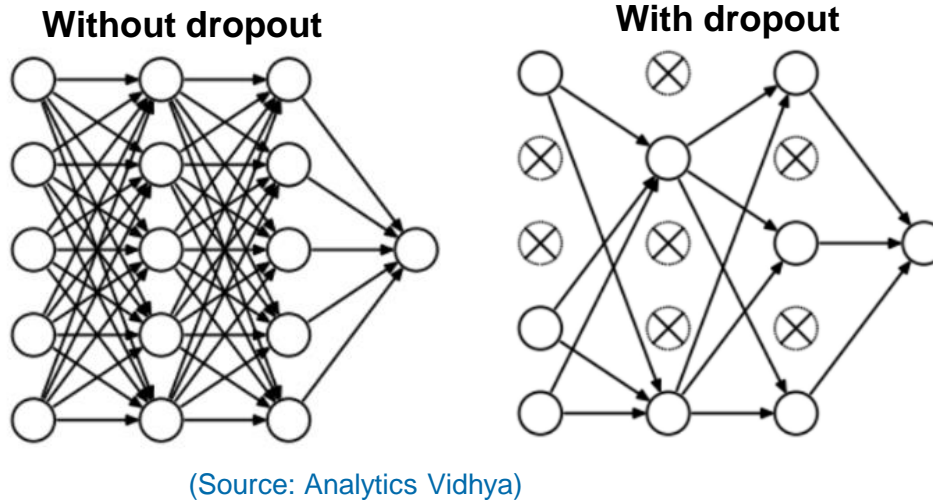
## Training Vs. Test Set Error





# Dropout

## Reduce Overfitting



- This is a **cheap technique** to reduce model capacity
  - Reduce overfitting
- In each iteration, at each layer, **randomly choose** some neurons and **drop all connections** from these neurons
  - $\text{dropout\_rate} = 1 - \text{keep\_prob}$



# Dropout

## Reduce Overfitting

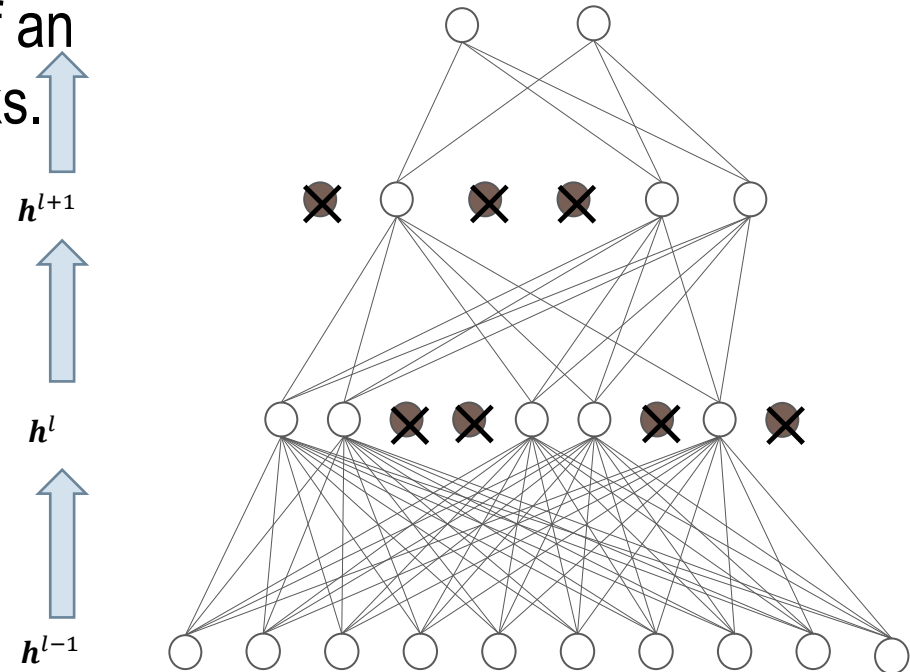
- Computationally efficient
- Can be considered a **bagged ensemble** of an exponential number ( $2^N$ ) of neural networks.

- **Training**

$$\begin{aligned} \mathbf{r} &\sim \text{Bernoulli}(\mu) \\ \tilde{\mathbf{h}}^l &= \mathbf{h}^l \odot \mathbf{r} \\ \mathbf{h}^{l+1} &= \sigma(W^{(l)\top} \tilde{\mathbf{h}}^l + \mathbf{b}^l) \end{aligned}$$

- **Testing**

- No dropout (dropout\_rate = 0).





# Internal covariate shift problem

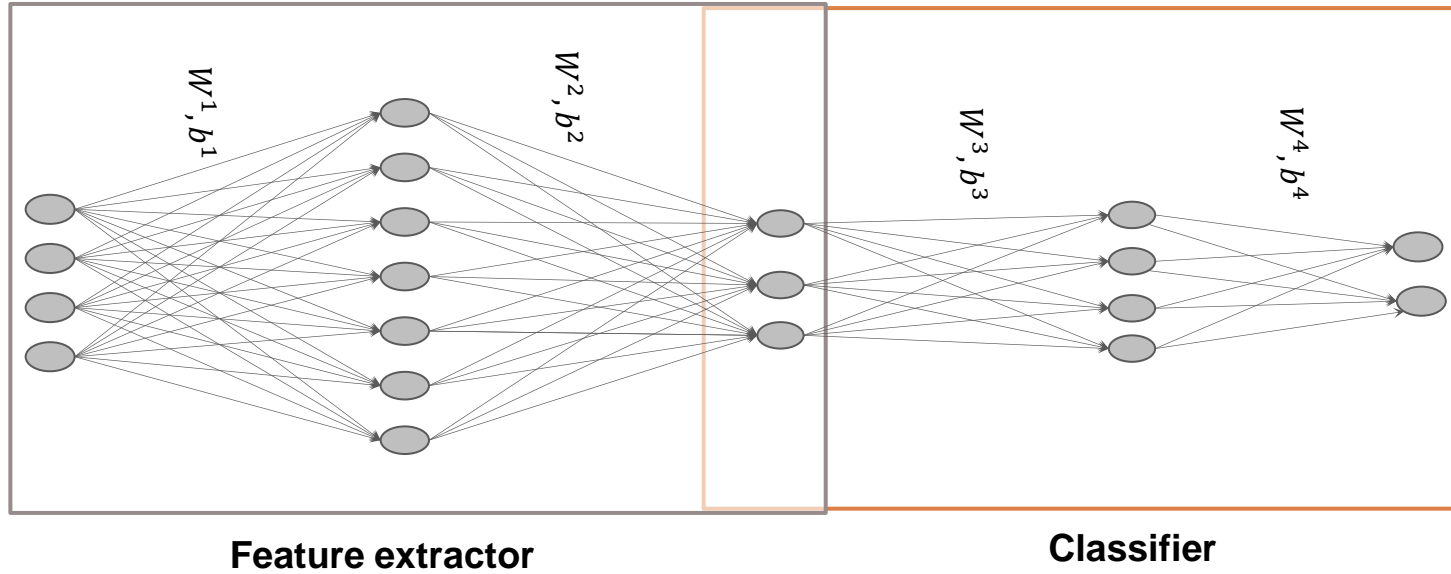
Input batch

|         |         |         |         |
|---------|---------|---------|---------|
| $x_1^1$ | $x_2^1$ | $x_3^1$ | $x_4^1$ |
| $x_1^2$ | $x_2^2$ | $x_3^2$ | $x_4^2$ |
| $x_1^3$ | $x_2^3$ | $x_3^3$ | $x_4^3$ |
| $x_1^4$ | $x_2^4$ | $x_3^4$ | $x_4^4$ |



Representation batch

|         |         |         |
|---------|---------|---------|
| $z_1^1$ | $z_2^1$ | $z_3^1$ |
| $z_1^2$ | $z_2^2$ | $z_3^2$ |
| $z_1^3$ | $z_2^3$ | $z_3^3$ |
| $z_1^4$ | $z_2^4$ | $z_3^4$ |



**Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift**

Sergey Ioffe  
Christian Szegedy

Google, 1600 Amphitheatre Pkwy, Mountain View, CA 94043

SIOFFE@GOOGLE.COM  
SZEGEDY@GOOGLE.COM

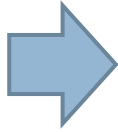
Paper link: <http://proceedings.mlr.press/v37/ioffe15.pdf>



# Internal covariate shift problem

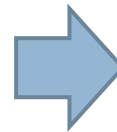
Input batch 1

|         |         |         |         |
|---------|---------|---------|---------|
| $x_1^1$ | $x_2^1$ | $x_3^1$ | $x_4^1$ |
| $x_1^2$ | $x_2^2$ | $x_3^2$ | $x_4^2$ |
| $x_1^3$ | $x_2^3$ | $x_3^3$ | $x_4^3$ |
| $x_1^4$ | $x_2^4$ | $x_3^4$ | $x_4^4$ |



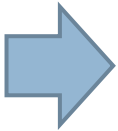
Representation batch 1

|         |         |         |
|---------|---------|---------|
| $z_1^1$ | $z_2^1$ | $z_3^1$ |
| $z_1^2$ | $z_2^2$ | $z_3^2$ |
| $z_1^3$ | $z_2^3$ | $z_3^3$ |
| $z_1^4$ | $z_2^4$ | $z_3^4$ |



Input batch 2

|         |         |         |         |
|---------|---------|---------|---------|
| $x_1^5$ | $x_2^5$ | $x_3^5$ | $x_4^5$ |
| $x_1^6$ | $x_2^6$ | $x_3^6$ | $x_4^6$ |
| $x_1^7$ | $x_2^7$ | $x_3^7$ | $x_4^7$ |
| $x_1^8$ | $x_2^8$ | $x_3^8$ | $x_4^8$ |



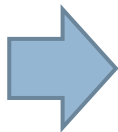
Representation batch 2

|         |         |         |
|---------|---------|---------|
| $z_1^5$ | $z_2^5$ | $z_3^5$ |
| $z_1^6$ | $z_2^6$ | $z_3^6$ |
| $z_1^7$ | $z_2^7$ | $z_3^7$ |
| $z_1^8$ | $z_2^8$ | $z_3^8$ |



Input batch 3

|            |            |            |            |
|------------|------------|------------|------------|
| $x_1^9$    | $x_2^9$    | $x_3^9$    | $x_4^9$    |
| $x_1^{10}$ | $x_2^{10}$ | $x_3^{10}$ | $x_4^{10}$ |
| $x_1^{11}$ | $x_2^{11}$ | $x_3^{11}$ | $x_4^{11}$ |
| $x_1^{12}$ | $x_2^{12}$ | $x_3^{12}$ | $x_4^{12}$ |



Representation batch 3

|            |            |            |
|------------|------------|------------|
| $z_1^9$    | $z_2^9$    | $z_3^9$    |
| $z_1^{10}$ | $z_2^{10}$ | $z_3^{10}$ |
| $z_1^{11}$ | $z_2^{11}$ | $z_3^{11}$ |
| $z_1^{12}$ | $z_2^{12}$ | $z_3^{12}$ |

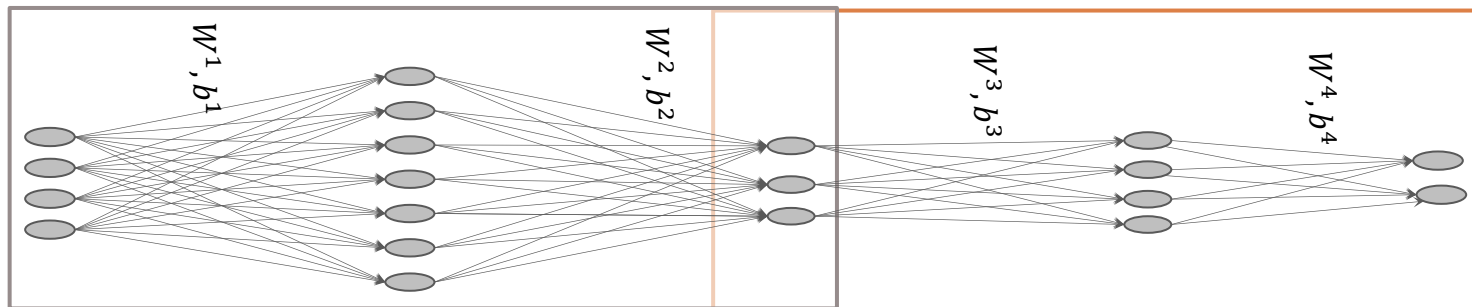


difference

difference

□ **Internal** covariate shift problem:

- Significant difference in statistics of input batches and also representation batches.
- Statistical differences among mini-batches make the classifier harder to learn from data.

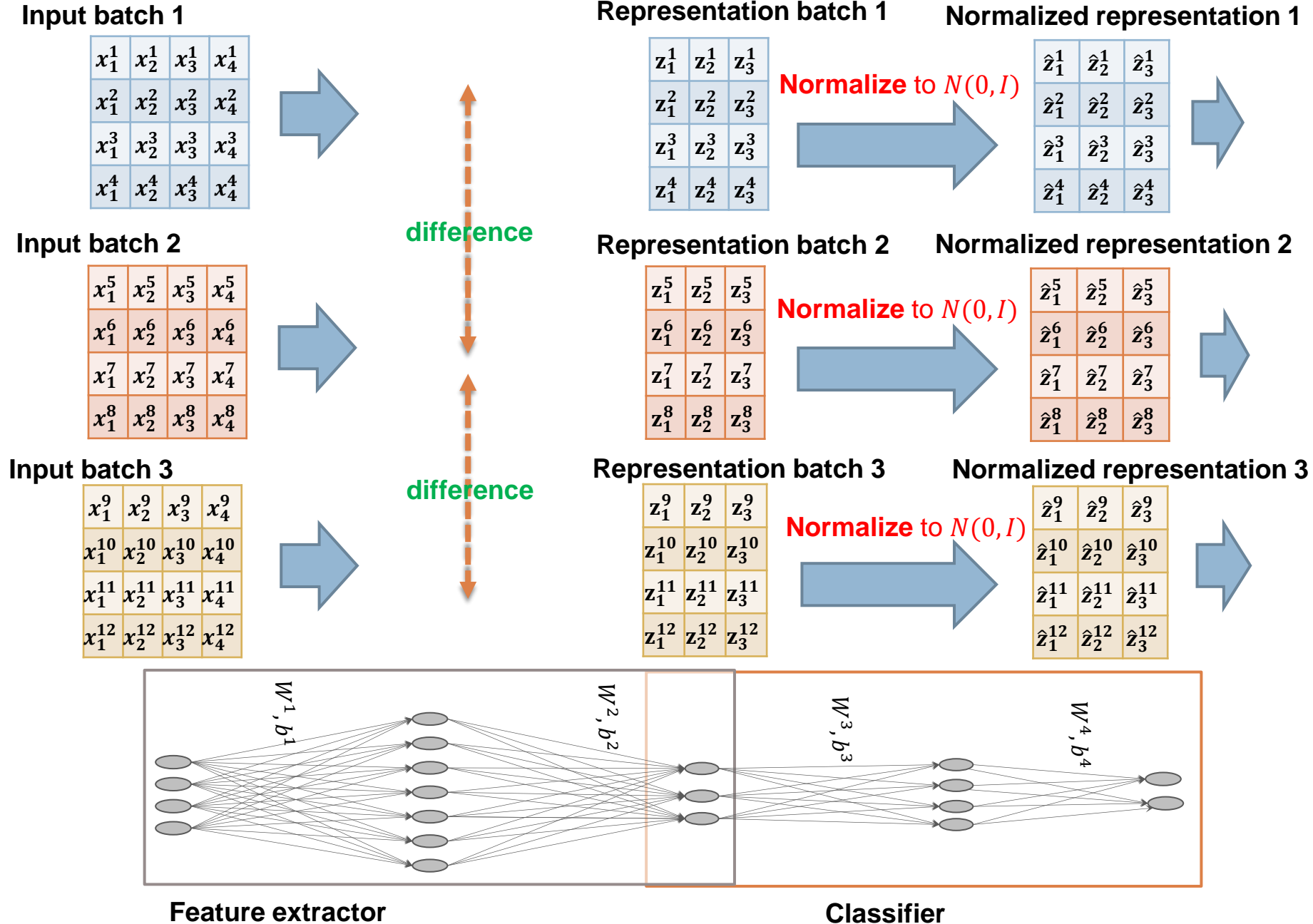


Feature extractor

Classifier

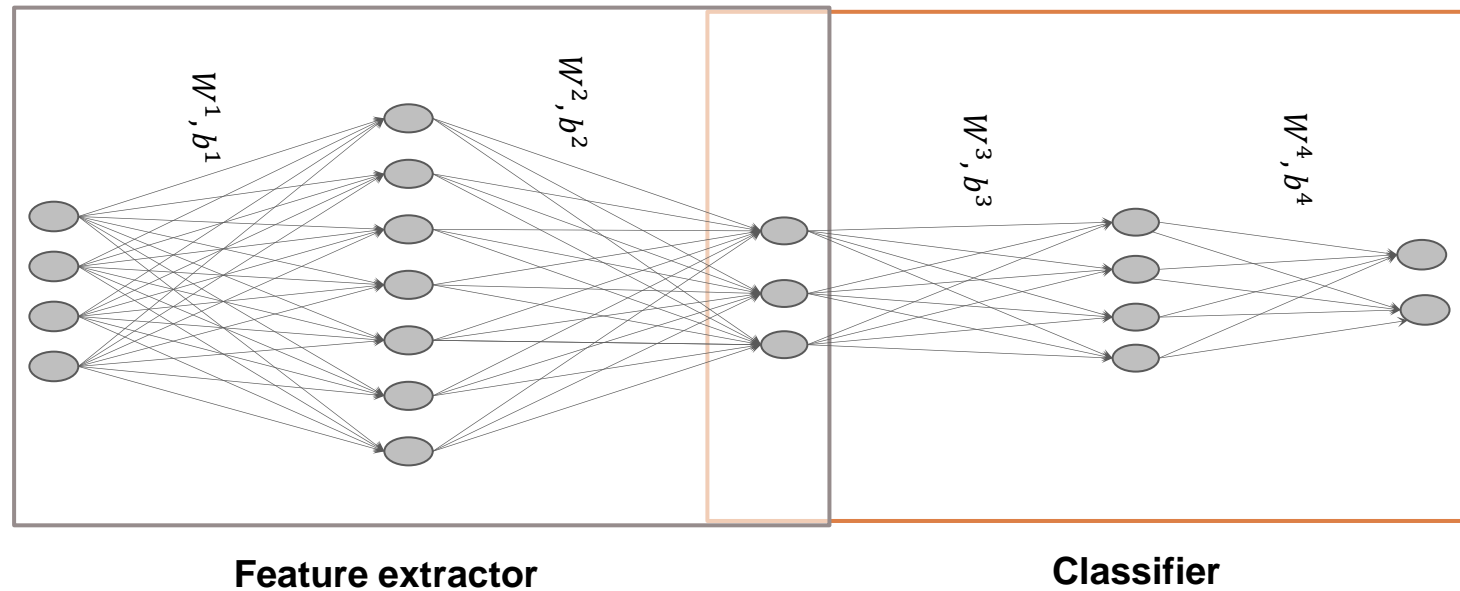
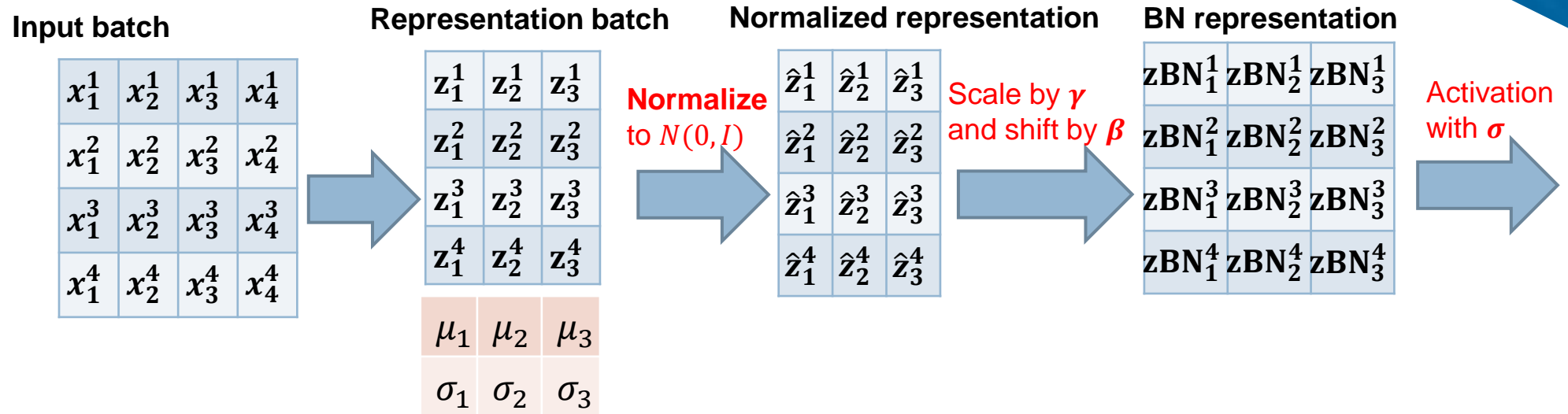


# Batch Normalization





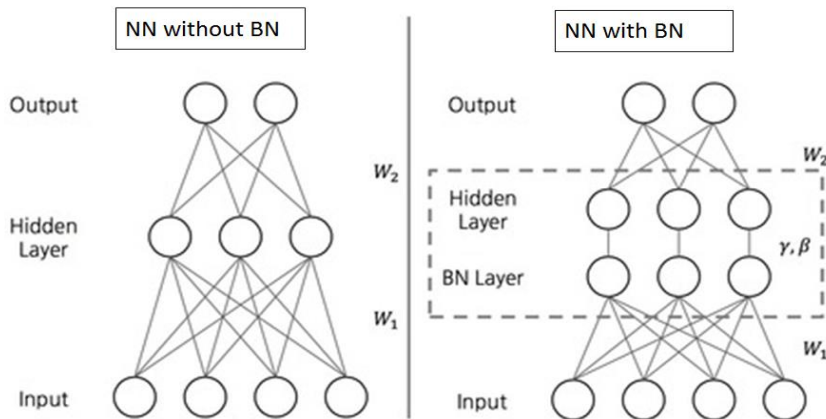
# Batch Normalization



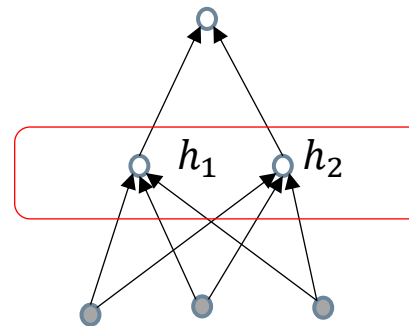


# Batch Normalization

1. Cope with internal covariate shift
2. Reduce gradient vanishing/exploding
3. Reduce overfitting
4. Make training more stable
5. Converge faster
  1. Allow us to train with bigger learning rate



- Let  $z = W^k h^k + b^k$  be the mini-batch before activation. We compute the normalized  $\hat{z}$  as
  - $\hat{z} = \frac{z - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$  where  $\epsilon$  is a small value such as  $1e^{-7}$
  - $\mu_B = \frac{1}{b} \sum_{i=1}^b z_i$  is the empirical mean
  - $\sigma_B^2 = \frac{1}{b} \sum_{i=1}^b (z_i - \mu_B)^2$  is the empirical variance
- We scale the normalized  $\hat{z}$ 
  - $z_{BN} = \gamma \hat{z} + \beta$  where  $\gamma, \beta > 0$  are two learnable parameters (i.e., scale and shift parameters)
- We then apply the activation to obtain the next layer value
  - $h^{k+1} = \sigma(z_{BN})$



| $z_1$ | $z_2$ |
|-------|-------|
| 0.1   | 0.2   |
| ...   | ...   |
| 0.5   | 0.4   |

Mini-batch size

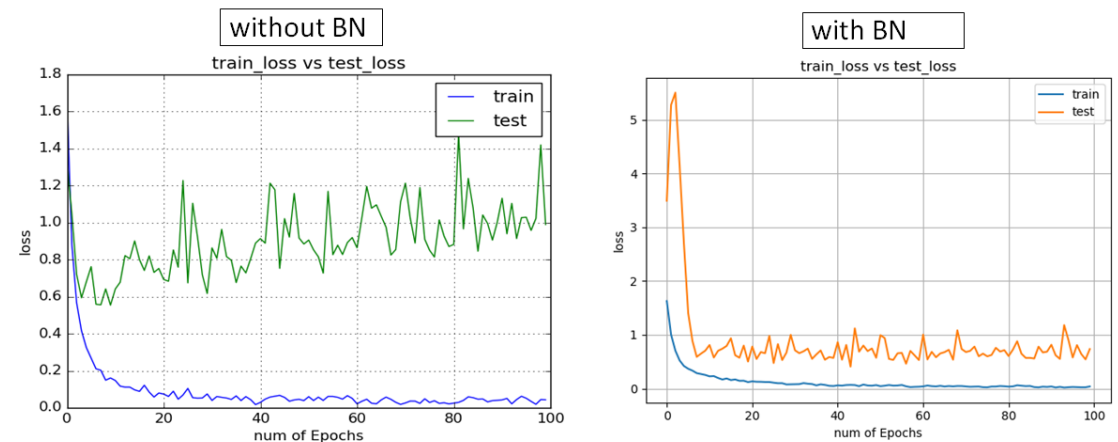
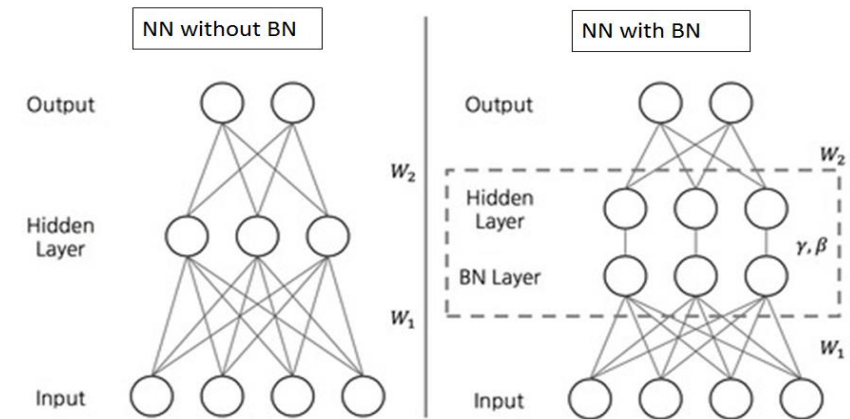
Standardize column-wise



# Batch Normalization

## Testing Phase

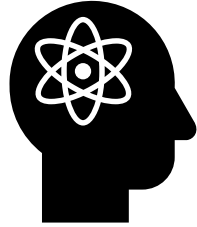
- At testing time, let's say we only want to test on a single input  $x$
- Hence, we don't have a set of mini-batch samples to compute mean and standard deviation.
- So, we replace the mini-batch  $\mu_B$  and  $\sigma_B$  with running averages of  $\tilde{\mu}_B$  and  $\tilde{\sigma}_B$  computed during the training process.
  - $\tilde{\mu}_B = \theta \tilde{\mu}_B + (1 - \theta) \mu_B$
  - $\tilde{\sigma}_B = \theta \tilde{\sigma}_B + (1 - \theta) \sigma_B$
  - $0 < \theta < 1$  is the momentum decay (i.e.,  $\theta = 0.9$ ).



(Source: medium.com)

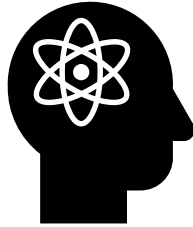


# Data Augmentation



## Reality

- You have a **tiny dataset** of **10K images**, and you need to train a **good deep net**.



What are the **criteria** of a **qualified training set**?

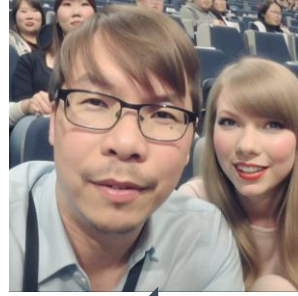
### Quantity?

- Collect **more** and **more data**?

### Quality?

- More **diverge** data?
- More **qualified** data?

Data Augmentation



Prof Dinh Phung









Create many variants

| Original   | Flip  | Rotation   | Random crop   |
|--|---|--|---|
|  |   |  |   |
| <ul style="list-style-type: none"><li>Image without any modification</li></ul>   | <ul style="list-style-type: none"><li>Flipped with respect to an axis for which the meaning of the image is preserved</li></ul> | <ul style="list-style-type: none"><li>Rotation with a slight angle</li><li>Simulates incorrect horizon calibration</li></ul> | <ul style="list-style-type: none"><li>Random focus on one part of the image</li><li>Several random crops can be done in a row</li></ul> |
| Color shift  | Noise addition  | Information loss   | Contrast change   |
|  |   |  |   |
| <ul style="list-style-type: none"><li>Nuances of RGB is slightly changed</li><li>Captures noise that can occur with light exposure</li></ul> | <ul style="list-style-type: none"><li>Addition of noise</li><li>More tolerance to quality variation of inputs</li></ul>         | <ul style="list-style-type: none"><li>Parts of image ignored</li><li>Mimics potential loss of parts of image</li></ul>       | <ul style="list-style-type: none"><li>Luminosity changes</li><li>Controls difference in exposition due to time of day</li></ul>         |



# Data Augmentation

- Use **simple transformations** to augment data examples. Models will be **challenged** with **diverge data examples** which might be **encountered** in the testing set
  - Rotation, Width Shifting, Height Shifting, Brightness, Shear Intensity, Zoom, Channel Shift, Horizontal Flip, Vertical Flip
- This will **reduce overfitting**, making this a **regularization technique**. The trick is to **generate realistic training instances**

| Original  | Flip  | Rotation  | Random crop  |
|---|---|---|--|
|    |    |    |   |
| <ul style="list-style-type: none"> <li>• Image without any modification</li> </ul>  | <ul style="list-style-type: none"> <li>• Flipped with respect to an axis for which the meaning of the image is preserved</li> </ul> | <ul style="list-style-type: none"> <li>• Rotation with a slight angle</li> <li>• Simulates incorrect horizon calibration</li> </ul> | <ul style="list-style-type: none"> <li>• Random focus on one part of the image</li> <li>• Several random crops can be done in a row</li> </ul> |
| Color shift   | Noise addition  | Information loss  | Contrast change  |
|   |   |   |    |
| <ul style="list-style-type: none"> <li>• Nuances of RGB is slightly changed</li> <li>• Captures noise that can occur with light exposure</li> </ul> | <ul style="list-style-type: none"> <li>• Addition of noise</li> <li>• More tolerance to quality variation of inputs</li> </ul>      | <ul style="list-style-type: none"> <li>• Parts of image ignored</li> <li>• Mimics potential loss of parts of image</li> </ul>       | <ul style="list-style-type: none"> <li>• Luminosity changes</li> <li>• Controls difference in exposition due to time of day</li> </ul>         |

[Source: Stanford CS 230 Deep Learning]



# Data Augmentation in PyTorch

```
test_transform = transforms.Compose([transforms.ToTensor(),
                                    transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5)), # Normalize the images, each R,G,B value is normalized with mean=0.5 and std=0.5
                                    transforms.Resize((32,32)), #resizes the image so it can be perfect for our model.
                                    ])

train_transform = transforms.Compose([transforms.Resize((32,32)), #resizes the image so it can be perfect for our model.
                                     transforms.RandomHorizontalFlip(), # FLips the image w.r.t horizontal axis
                                     #transforms.RandomRotation(4), #Rotates the image to a specified angel
                                     #transforms.RandomAffine(0, shear=10, scale=(0.8,1.2)), #Performs actions like zooms, change shear angles.
                                     transforms.ColorJitter(brightness=0.2, contrast=0.2, saturation=0.2), # Set the color params
                                     transforms.ToTensor(), # convert the image to tensor so that it can work with torch
                                     transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5)), # Normalize the images, each R,G,B value is normalized with mean=0.5 and std=0.5
                                     ])

full_train_set = torchvision.datasets.CIFAR10("./data", download=True, transform=train_transform) # Apply train_transform to train set
full_valid_set = torchvision.datasets.CIFAR10("./data", download=True, transform=test_transform) # Apply test_transform to generate valid set
full_test_set = torchvision.datasets.CIFAR10("./data", download=True, train=False, transform=test_transform)

n_train, n_valid, n_test = 5000, 5000, 5000

total_num_train = len(full_train_set)
total_num_test = len(full_test_set)
train_valid_idx = torch.randperm(total_num_train)
train_set = torch.utils.data.Subset(full_train_set, train_valid_idx[:n_train])
valid_set = torch.utils.data.Subset(full_valid_set, train_valid_idx[n_train:n_train+n_valid])

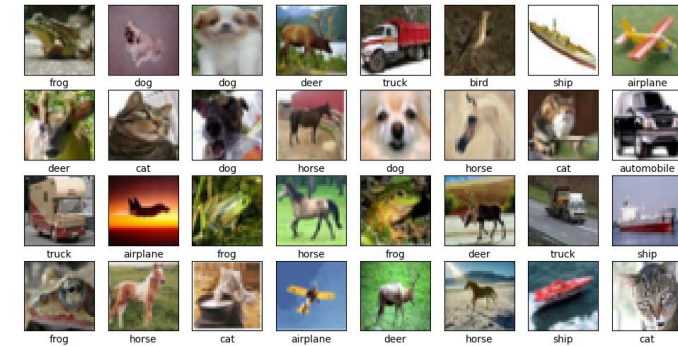
test_idx = torch.randperm(total_num_test)
test_set = torch.utils.data.Subset(full_test_set, test_idx[:n_test])

print("Traing set\n\t-Number of samples:\t{}\n\t-Shape of 1 sample:\t{}".format(len(train_set), list(train_set[0][0].shape)))
print("Valid set\n\t-Number of samples:\t{}\n\t-Shape of 1 sample:\t{}".format(len(valid_set), list(valid_set[0][0].shape)))
print("Test set\n\t-Number of samples:\t{}\n\t-Shape of 1 sample:\t{}".format(len(test_set), list(test_set[0][0].shape)))

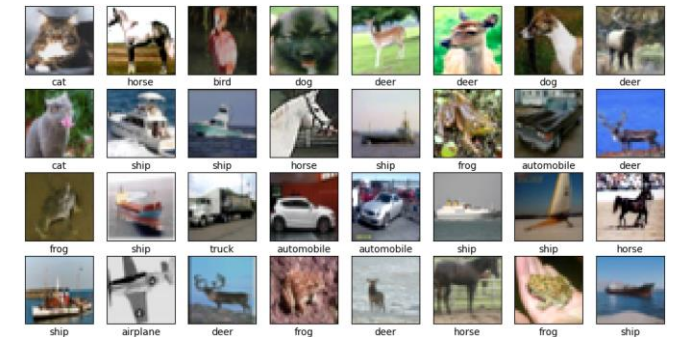
train_loader = torch.utils.data.DataLoader(train_set, batch_size=32, shuffle=True)
test_loader = torch.utils.data.DataLoader(test_set, batch_size=32)
valid_loader = torch.utils.data.DataLoader(valid_set, batch_size=32)

img_train = [train_set[idx][0].numpy().transpose((1,2,0)) for idx in range(32)]
label_train = [train_set[idx][1] for idx in range(32)]
```

## Without augmentation



## With augmentation









Some additional regularization techniques

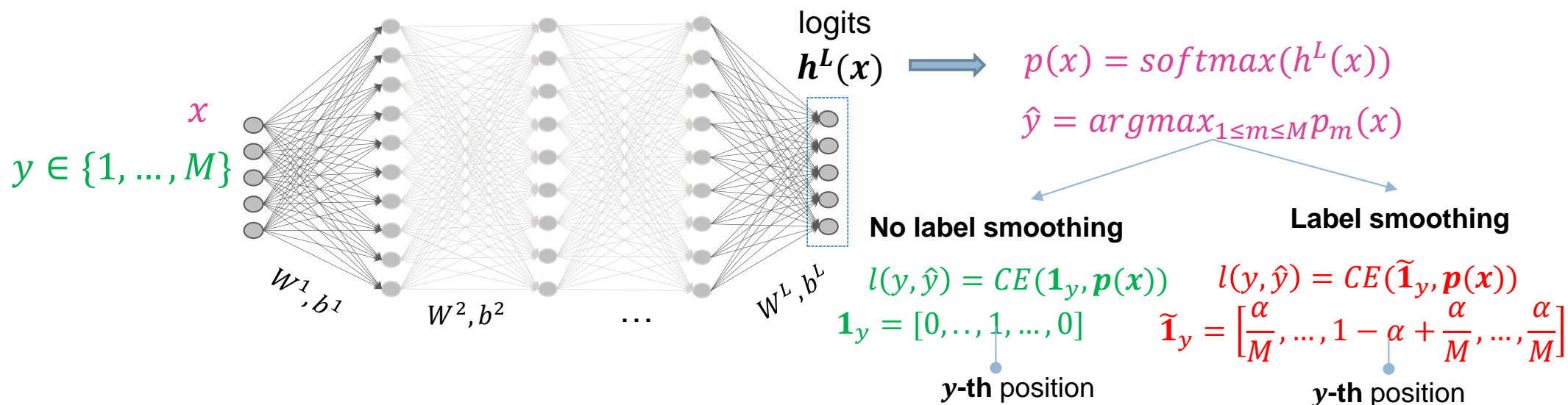


# Label smoothing

## When Does Label Smoothing Help?

Rafael Müller\*, Simon Kornblith, Geoffrey Hinton  
Google Brain  
Toronto  
rafaelmuller@google.com

Paper link: <https://papers.nips.cc/paper/2019/file/f1748d6b0fd9d439f71450117eba2725-Paper.pdf>



- Given data instance  $(x, y)$  with the label  $y \in \{1, \dots, M\}$ , we compute the **CE loss** between the prediction probabilities  $\mathbf{p}(x)$  and the smooth label

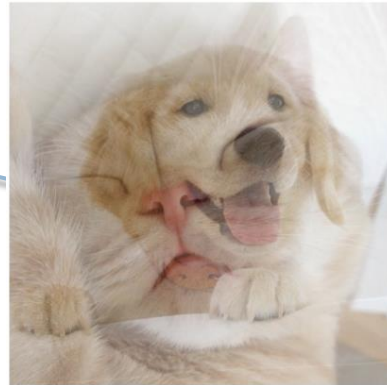
- $l(y, \hat{y}) = CE(\tilde{\mathbf{1}}_y, \mathbf{p}(x))$  with  $\tilde{\mathbf{1}}_y = (1 - \alpha) \times \mathbf{1}_y + \frac{\alpha}{M} \times \mathbf{1}$  where  $\mathbf{1}$  is a vector of all 1 and  $0 < \alpha < 1$ .



# Data mix-up



$(x_1, \mathbf{1}_{y_1})$



$$\lambda \sim \text{Beta}(\alpha, \alpha)$$

**Blended image**  $\tilde{x} = \lambda \times x_1 + (1 - \lambda) \times x_2$

**Blended label**  $\tilde{y} = \lambda \times \mathbf{1}_{y_1} + (1 - \lambda) \times \mathbf{1}_{y_2}$

↳ **min**  $CE(\tilde{y}, p(\tilde{x}))$



$(x_2, \mathbf{1}_{y_2})$

*mixup*: BEYOND EMPIRICAL RISK MINIMIZATION

Hongyi Zhang  
MIT

Moustapha Cisse, Yann N. Dauphin, David Lopez-Paz\*  
FAIR

Paper link: <https://openreview.net/pdf?id=r1Ddp1-Rb>

[Source: <https://medium.com/>]

□ for  $(x_1, y_1), (x_2, y_2)$  in zip(batch1, batch 2)

1.  $\lambda \sim \text{Beta}(\alpha, \alpha)$
2.  $\tilde{x} = \lambda \times x_1 + (1 - \lambda) \times x_2$
3.  $\tilde{y} = \lambda \times \mathbf{1}_{y_1} + (1 - \lambda) \times \mathbf{1}_{y_2}$
4. Update optimizer to minimize  $CE(\tilde{y}, p(\tilde{x}))$



# Cut-mix

[Source: <https://encord.com/blog/data-augmentation-guide/>]



$$(x_1, \mathbf{1}_{y_1}), x_1 \in \mathbb{R}^{C \times W \times H}$$

$$\lambda \sim \text{Beta}(\alpha, \alpha)$$

$$(x_2, \mathbf{1}_{y_2}), x_2 \in \mathbb{R}^{C \times W \times H}$$

$$\tilde{x} = M \odot x_1 + (1 - M) \odot x_2, M \in \{0, 1\}^{H \times W}$$

$$\tilde{y} = \lambda \times \mathbf{1}_{y_1} + (1 - \lambda) \times \mathbf{1}_{y_2}$$

$$\rightarrow \min \text{CE}(\tilde{y}, p(\tilde{x}))$$

for  $(x_1, y_1), (x_2, y_2)$  in zip(batch1, batch 2)

1.  $\lambda \sim \text{Beta}(\alpha, \alpha)$
2. Sample a **bounding box**  $B = [r_x, r_y, r_w, r_h]$ 
  1.  $r_x \sim \text{Uni}[0, W], r_w \sim W\sqrt{1 - \lambda}$
  2.  $r_y \sim \text{Uni}[0, H], r_h \sim H\sqrt{1 - \lambda}$
3.  $M \in \{0, 1\}^{W \times H}$  by filling 1 within B and 0 otherwise
4.  $\tilde{x} = M \odot x_1 + (1 - M) \odot x_2$
5. Update optimizer to minimize  $\text{CE}(\tilde{y}, p(\tilde{x}))$

## CutMix: Regularization Strategy to Train Strong Classifiers with Localizable Features

Sangdoo Yun<sup>1</sup>

Dongyoon Han<sup>1</sup>  
Junsuk Choe<sup>1,3</sup>

Seong Joon Oh<sup>2</sup>  
Youngjoon Yoo<sup>1</sup>

Sanghyuk Chun<sup>1</sup>

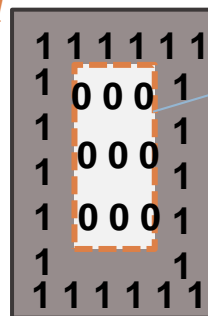
<sup>1</sup>Clova AI Research, NAVER Corp.

<sup>2</sup>Clova AI Research, LINE Plus Corp.

<sup>3</sup>Yonsei University

[Source: <https://arxiv.org/pdf/1905.04899>]

$M$



$$B = [r_x, r_y, r_w, r_h]$$

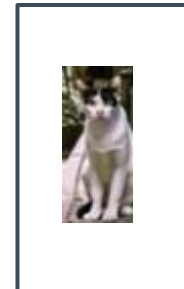
$$\frac{\text{area}(B)}{\text{area}(\text{image})} = \frac{WH(1 - \lambda)}{WH} = 1 - \lambda$$



$$\odot M =$$



$$\odot (1 - M) =$$









## Transfer learning and fine-tuning

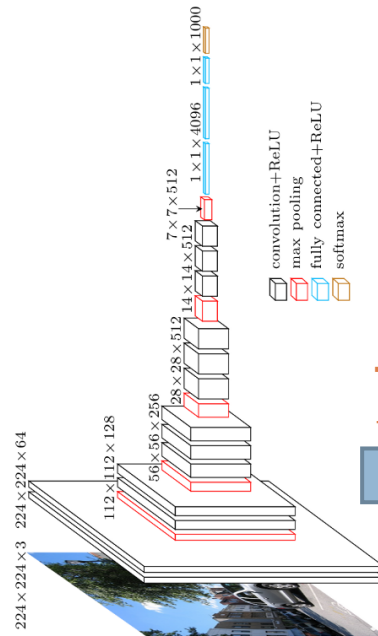


# Transfer Learning

## Motivation

### Large-scale dataset (ImageNet)

- over 1.2 million images and 1,000 possible object categories



Transfer learning  
+ Fine tune

### Your small-scale dataset (Flower-17)

- 17 category dataset with 80 images per class



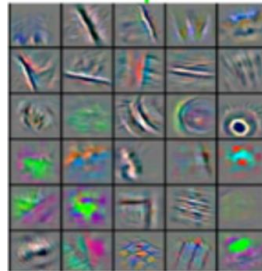
### Powerful pretrained model

- VGG16, VGG19
- Inception V3
- Xception
- ResNet

Not enough data to train  
a good model.  
HOW?



Low-level filers



Mid-level filers



High-level filers

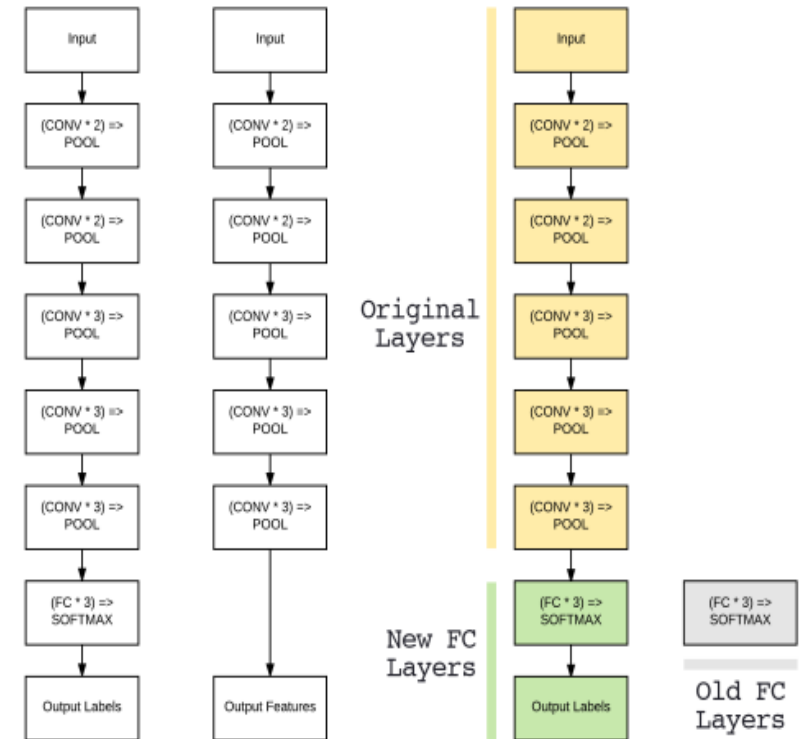
Fits the target  
dataset



# Transfer Learning

## How to Do That?

- **Remove** FC layers from the pretrained model
- **Replace** them with a brand-new FC head.
  - These new FC layers can then be fine-tuned to the specific dataset
  - The old FC layers are no longer used

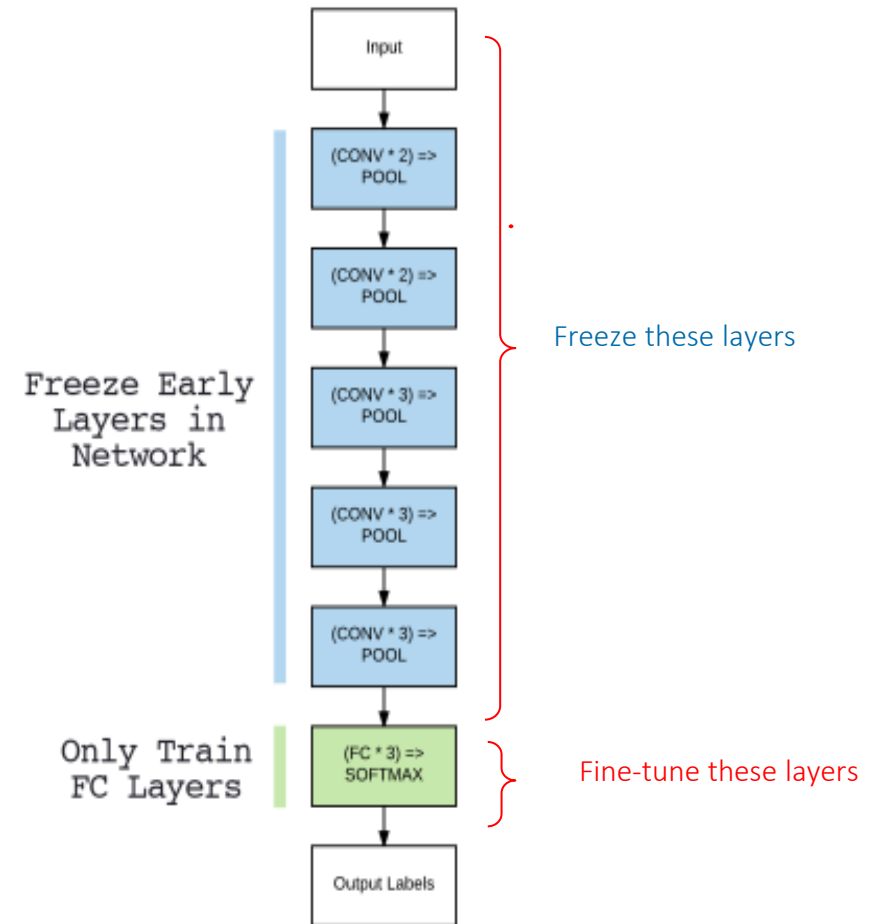




# Transfer Learning

## How to Do That?

- **Freeze** all CONV layers in the network
  - Only allow the gradient to backpropagate through the FC layers
  - Doing this allows our network to **warm up**
- Training data is forward propagated through the network
  - However, the backpropagation is stopped after the FC layers
  - Allows these layers to start to learn patterns from the highly discriminative CONV layers



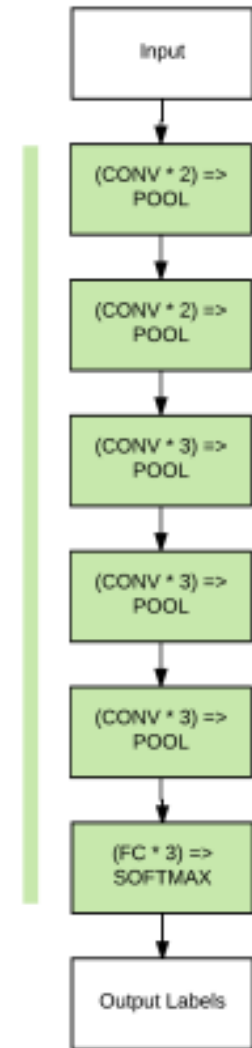


# Transfer Learning

## How to Do That?

- ❑ After the FC layers have had a chance to warm up, we may choose to **unfreeze** all layers in the network
  - ❑ Allow each of them to be **fine-tuned**.
  - ❑ Continue training the entire network, *but with a **very small learning rate***
  - ❑ We do not want to **deviate our CONV filters** dramatically. Training is then allowed to continue until sufficient accuracy is obtained.

Unfreeze Early  
Layers & Train  
All





# Model zoo supported by PyTorch

| Model                           | Acc@1  | Acc@5  |
|---------------------------------|--------|--------|
| AlexNet                         | 56.522 | 79.066 |
| VGG-11                          | 69.020 | 88.628 |
| VGG-13                          | 69.928 | 89.246 |
| VGG-16                          | 71.592 | 90.382 |
| VGG-19                          | 72.376 | 90.876 |
| VGG-11 with batch normalization | 70.370 | 89.810 |
| VGG-13 with batch normalization | 71.586 | 90.374 |
| VGG-16 with batch normalization | 73.360 | 91.516 |
| VGG-19 with batch normalization | 74.218 | 91.842 |
| ResNet-18                       | 69.758 | 89.078 |
| ResNet-34                       | 73.314 | 91.420 |
| ResNet-50                       | 76.130 | 92.862 |
| ResNet-101                      | 77.374 | 93.546 |
| ResNet-152                      | 78.312 | 94.046 |
| SqueezeNet 1.0                  | 58.092 | 80.420 |
| SqueezeNet 1.1                  | 58.178 | 80.624 |
| Densenet-121                    | 74.434 | 91.972 |

|                    |        |        |
|--------------------|--------|--------|
| Densenet-169       | 75.600 | 92.806 |
| Densenet-201       | 76.896 | 93.370 |
| Densenet-161       | 77.138 | 93.560 |
| Inception v3       | 77.294 | 93.450 |
| GoogLeNet          | 69.778 | 89.530 |
| ShuffleNet V2 x1.0 | 69.362 | 88.316 |
| ShuffleNet V2 x0.5 | 60.552 | 81.746 |
| MobileNet V2       | 71.878 | 90.286 |
| MobileNet V3 Large | 74.042 | 91.340 |
| MobileNet V3 Small | 67.668 | 87.402 |
| ResNeXt-50-32x4d   | 77.618 | 93.698 |
| ResNeXt-101-32x8d  | 79.312 | 94.526 |
| Wide ResNet-50-2   | 78.468 | 94.086 |
| Wide ResNet-101-2  | 78.848 | 94.284 |
| MNASNet 1.0        | 73.456 | 91.510 |
| MNASNet 0.5        | 67.734 | 87.490 |



# Transfer learning with PyTorch

```
VGG(
  (features): Sequential(
    (0): Conv2d(3, 64, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (1): ReLU(inplace=True)
    (2): Conv2d(64, 64, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (3): ReLU(inplace=True)
    (4): MaxPool2d(kernel_size=2, stride=2, padding=0, dilation=1, ceil_mode=False)
    (5): Conv2d(64, 128, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (6): ReLU(inplace=True)
    (7): Conv2d(128, 128, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (8): ReLU(inplace=True)
    (9): MaxPool2d(kernel_size=2, stride=2, padding=0, dilation=1, ceil_mode=False)
    (10): Conv2d(128, 256, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (11): ReLU(inplace=True)
    (12): Conv2d(256, 256, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (13): ReLU(inplace=True)
    (14): Conv2d(256, 256, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (15): ReLU(inplace=True)
    (16): Conv2d(256, 256, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (17): ReLU(inplace=True)
    (18): MaxPool2d(kernel_size=2, stride=2, padding=0, dilation=1, ceil_mode=False)
    (19): Conv2d(256, 512, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (20): ReLU(inplace=True)
    (21): Conv2d(512, 512, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (22): ReLU(inplace=True)
    (23): Conv2d(512, 512, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (24): ReLU(inplace=True)
    (25): Conv2d(512, 512, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (26): ReLU(inplace=True)
    (27): MaxPool2d(kernel_size=2, stride=2, padding=0, dilation=1, ceil_mode=False)
    (28): Conv2d(512, 512, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (29): ReLU(inplace=True)
    (30): Conv2d(512, 512, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (31): ReLU(inplace=True)
    (32): Conv2d(512, 512, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (33): ReLU(inplace=True)
    (34): Conv2d(512, 512, kernel_size=(3, 3), stride=(1, 1), padding=(1, 1))
    (35): ReLU(inplace=True)
    (36): MaxPool2d(kernel_size=2, stride=2, padding=0, dilation=1, ceil_mode=False)
  )
  (avgpool): AdaptiveAvgPool2d(output_size=(7, 7))
  (classifier): Sequential(
    (0): Linear(in_features=25088, out_features=4096, bias=True)
    (1): ReLU(inplace=True)
    (2): Dropout(p=0.5, inplace=False)
    (3): Linear(in_features=4096, out_features=4096, bias=True)
    (4): ReLU(inplace=True)
    (5): Dropout(p=0.5, inplace=False)
    (6): Linear(in_features=4096, out_features=1000, bias=True)
  )
)
```

| Layer (type)                  | Output Shape        | Param #     |
|-------------------------------|---------------------|-------------|
| Conv2d-1                      | [-1, 64, 224, 224]  | 1,792       |
| ReLU-2                        | [-1, 64, 224, 224]  | 0           |
| Conv2d-3                      | [-1, 64, 224, 224]  | 36,928      |
| ReLU-4                        | [-1, 64, 224, 224]  | 0           |
| MaxPool2d-5                   | [-1, 64, 112, 112]  | 0           |
| Conv2d-6                      | [-1, 128, 112, 112] | 73,856      |
| ReLU-7                        | [-1, 128, 112, 112] | 0           |
| Conv2d-8                      | [-1, 128, 112, 112] | 147,584     |
| ReLU-9                        | [-1, 128, 112, 112] | 0           |
| MaxPool2d-10                  | [-1, 128, 56, 56]   | 0           |
| Conv2d-11                     | [-1, 256, 56, 56]   | 295,168     |
| ReLU-12                       | [-1, 256, 56, 56]   | 0           |
| Conv2d-13                     | [-1, 256, 56, 56]   | 590,080     |
| ReLU-14                       | [-1, 256, 56, 56]   | 0           |
| Conv2d-15                     | [-1, 256, 56, 56]   | 590,080     |
| ReLU-16                       | [-1, 256, 56, 56]   | 0           |
| Conv2d-17                     | [-1, 256, 56, 56]   | 590,080     |
| ReLU-18                       | [-1, 256, 56, 56]   | 0           |
| MaxPool2d-19                  | [-1, 256, 28, 28]   | 0           |
| Conv2d-20                     | [-1, 512, 28, 28]   | 1,180,160   |
| ReLU-21                       | [-1, 512, 28, 28]   | 0           |
| Conv2d-22                     | [-1, 512, 28, 28]   | 2,359,808   |
| ReLU-23                       | [-1, 512, 28, 28]   | 0           |
| Conv2d-24                     | [-1, 512, 28, 28]   | 2,359,808   |
| ReLU-25                       | [-1, 512, 28, 28]   | 0           |
| Conv2d-26                     | [-1, 512, 28, 28]   | 2,359,808   |
| ReLU-27                       | [-1, 512, 28, 28]   | 0           |
| MaxPool2d-28                  | [-1, 512, 14, 14]   | 0           |
| Conv2d-29                     | [-1, 512, 14, 14]   | 2,359,808   |
| ReLU-30                       | [-1, 512, 14, 14]   | 0           |
| Conv2d-31                     | [-1, 512, 14, 14]   | 2,359,808   |
| ReLU-32                       | [-1, 512, 14, 14]   | 0           |
| Conv2d-33                     | [-1, 512, 14, 14]   | 2,359,808   |
| ReLU-34                       | [-1, 512, 14, 14]   | 0           |
| Conv2d-35                     | [-1, 512, 14, 14]   | 2,359,808   |
| ReLU-36                       | [-1, 512, 14, 14]   | 0           |
| MaxPool2d-37                  | [-1, 512, 7, 7]     | 0           |
| AdaptiveAvgPool2d-38          | [-1, 512, 7, 7]     | 0           |
| Linear-39                     | [-1, 4096]          | 102,764,544 |
| ReLU-40                       | [-1, 4096]          | 0           |
| Dropout-41                    | [-1, 4096]          | 0           |
| Linear-42                     | [-1, 4096]          | 16,781,312  |
| ReLU-43                       | [-1, 4096]          | 0           |
| Dropout-44                    | [-1, 4096]          | 0           |
| Linear-45                     | [-1, 1000]          | 4,097,000   |
| Total params: 143,667,240     |                     |             |
| Trainable params: 143,667,240 |                     |             |

Will be replaced by a fresh new linear layer



# Transfer learning with PyTorch

## Warm-up the fresh new linear layer

```
# Freeze all layers
for param in model.parameters():
    param.requires_grad = False

# Modify the last fully connected layer for Flower102
num_features = model.classifier[6].in_features
model.classifier[6] = nn.Linear(num_features, 102)
model = model.to(device)

criterion = nn.CrossEntropyLoss()
optimizer = torch.optim.SGD(model.parameters(), lr=1e-3, momentum=0.9)
trainer = BaseTrainer(model, criterion, optimizer, train_loader, val_loader)
trainer.fit(num_epochs=10)
```

```
Epoch 1/10
  train_loss: 0.9840 - train_accuracy: 0.7027 - val_loss: 0.4316 - top1_acc: 0.8501 - top5_acc: 1.0000
Epoch 2/10
  train_loss: 0.4744 - train_accuracy: 0.8287 - val_loss: 0.3686 - top1_acc: 0.8706 - top5_acc: 1.0000
Epoch 3/10
  train_loss: 0.4272 - train_accuracy: 0.8505 - val_loss: 0.3627 - top1_acc: 0.8760 - top5_acc: 1.0000
Epoch 4/10
  train_loss: 0.3894 - train_accuracy: 0.8535 - val_loss: 0.3507 - top1_acc: 0.8787 - top5_acc: 1.0000
Epoch 5/10
  train_loss: 0.3738 - train_accuracy: 0.8631 - val_loss: 0.3283 - top1_acc: 0.8937 - top5_acc: 1.0000
Epoch 6/10
  train_loss: 0.3593 - train_accuracy: 0.8719 - val_loss: 0.3252 - top1_acc: 0.8815 - top5_acc: 1.0000
Epoch 7/10
  train_loss: 0.3309 - train_accuracy: 0.8886 - val_loss: 0.3134 - top1_acc: 0.8910 - top5_acc: 1.0000
Epoch 8/10
  train_loss: 0.3180 - train_accuracy: 0.8903 - val_loss: 0.3070 - top1_acc: 0.8924 - top5_acc: 1.0000
Epoch 9/10
  train_loss: 0.3062 - train_accuracy: 0.8917 - val_loss: 0.3121 - top1_acc: 0.8978 - top5_acc: 1.0000
Epoch 10/10
  train_loss: 0.3139 - train_accuracy: 0.8849 - val_loss: 0.3082 - top1_acc: 0.8924 - top5_acc: 1.0000
```

## Fine-tune the entire model

```
# Unfreeze the last convolutional block
# for param in model.features[-7:].parameters():
#     param.requires_grad = True

# Unfreeze model parameter
for param in model.parameters():
    param.requires_grad = True

criterion = nn.CrossEntropyLoss()
optimizer = torch.optim.SGD(model.parameters(), lr=1e-4, momentum=0.9)
trainer = BaseTrainer(model, criterion, optimizer, train_loader, val_loader)
trainer.fit(num_epochs=10)
```

```
Epoch 1/10
  train_loss: 0.2559 - train_accuracy: 0.9114 - val_loss: 0.2631 - top1_acc: 0.9101 - top5_acc: 1.0000
Epoch 2/10
  train_loss: 0.1983 - train_accuracy: 0.9305 - val_loss: 0.2489 - top1_acc: 0.9196 - top5_acc: 1.0000
Epoch 3/10
  train_loss: 0.1561 - train_accuracy: 0.9472 - val_loss: 0.2435 - top1_acc: 0.9196 - top5_acc: 1.0000
Epoch 4/10
  train_loss: 0.1417 - train_accuracy: 0.9513 - val_loss: 0.2349 - top1_acc: 0.9210 - top5_acc: 1.0000
Epoch 5/10
  train_loss: 0.1089 - train_accuracy: 0.9632 - val_loss: 0.2379 - top1_acc: 0.9223 - top5_acc: 1.0000
Epoch 6/10
  train_loss: 0.0947 - train_accuracy: 0.9690 - val_loss: 0.2370 - top1_acc: 0.9223 - top5_acc: 1.0000
Epoch 7/10
  train_loss: 0.0865 - train_accuracy: 0.9690 - val_loss: 0.2356 - top1_acc: 0.9319 - top5_acc: 1.0000
Epoch 8/10
  train_loss: 0.0644 - train_accuracy: 0.9816 - val_loss: 0.2403 - top1_acc: 0.9319 - top5_acc: 1.0000
Epoch 9/10
  train_loss: 0.0516 - train_accuracy: 0.9816 - val_loss: 0.2477 - top1_acc: 0.9319 - top5_acc: 1.0000
Epoch 10/10
  train_loss: 0.0530 - train_accuracy: 0.9837 - val_loss: 0.2477 - top1_acc: 0.9251 - top5_acc: 1.0000
```



# Summary

- Setting of a machine learning problem
  - General loss versus empirical loss
- Gradient vanishing/exploding and network initialization.
- Overfitting and underfitting
- Recipe for overfitting
  - Use regularization term
  - Dropout, batch norm
  - Data augmentation
  - Transfer learning
  - Label smoothing, data mix-up



# Thanks for your attention!

## Question time

