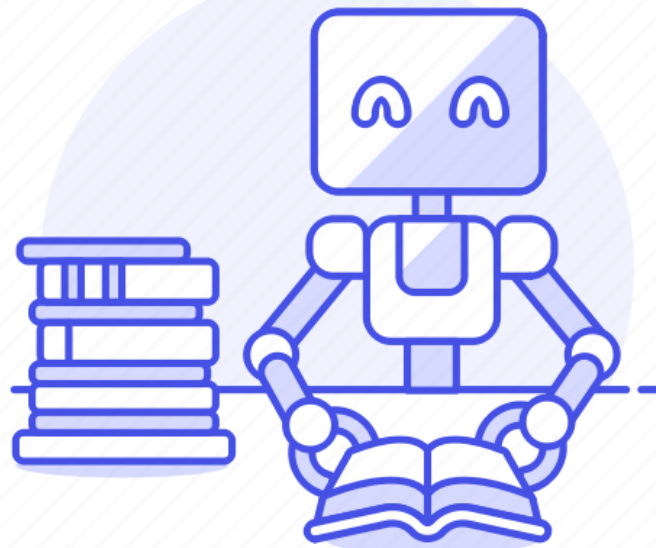


# L3 Introduction to Machine Learning

Zonghua Gu 2021

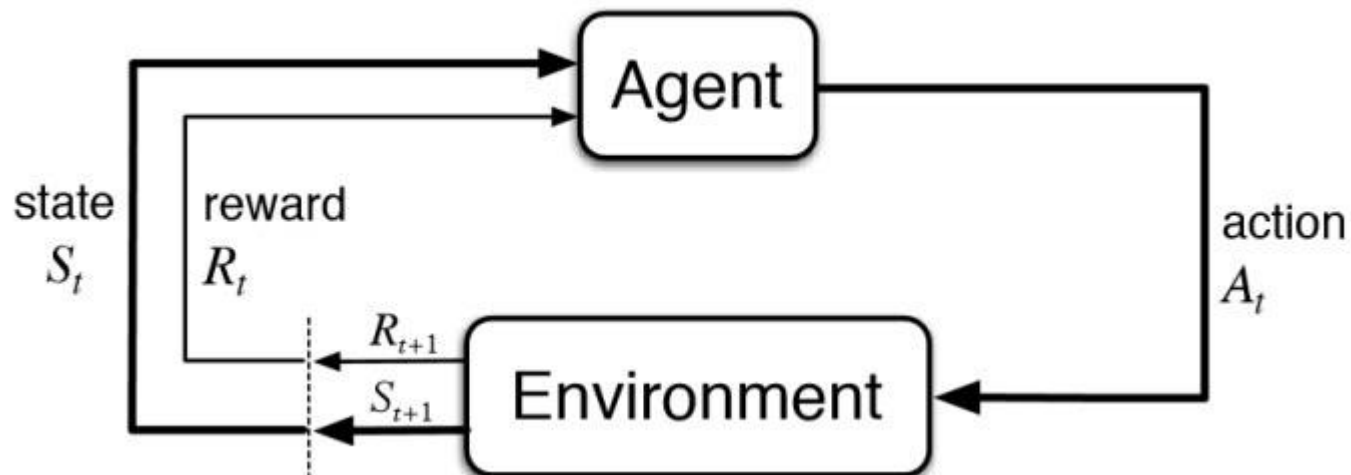


# ML Taxonomy

- Supervised Learning:
  - The system is presented with example inputs and their desired outputs, given by a “teacher”, and the goal is to learn a general rule that maps inputs to outputs.
    - Classification (cat or dog?)
    - Regression (housing price next year?)
- Unsupervised Learning:
  - No labels are given to the learning algorithm, leaving it on its own to find structure in its input. Unsupervised learning can be a goal in itself (discovering hidden patterns in data) or a means towards an end (feature learning).
    - Parametric UL (e.g., Gaussian Mixture Models)
    - Non-parametric UL

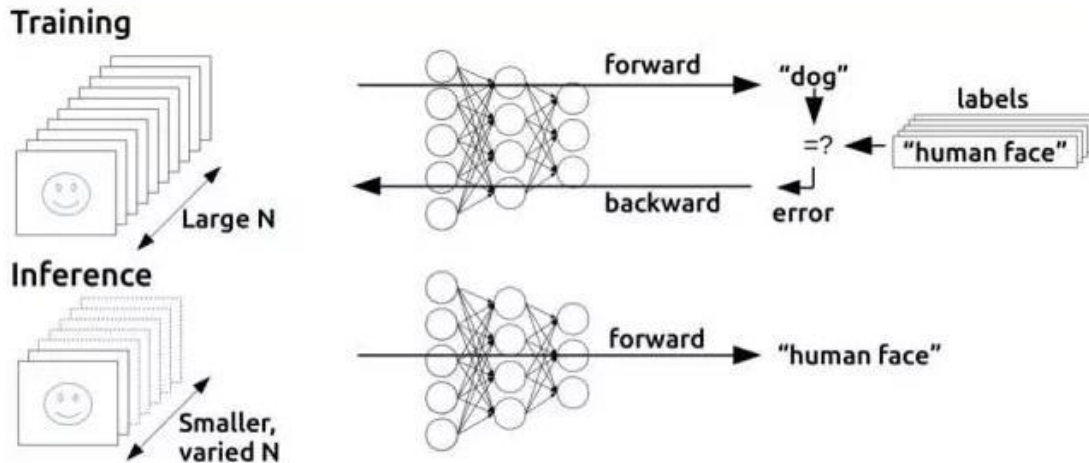
# ML Taxonomy

- Reinforcement Learning:
  - An agent interacts with a dynamic environment in which it must perform a certain goal. The agent is provided feedback in terms of rewards and it tries to learn an optimal policy that maximizes its cumulative rewards.
  - Algorithms: Model-based; Model-free (Value-based, Policy-based)
  - Applications: Game playing (AlphaGo); Robotics; AD...



# Training vs. Inference

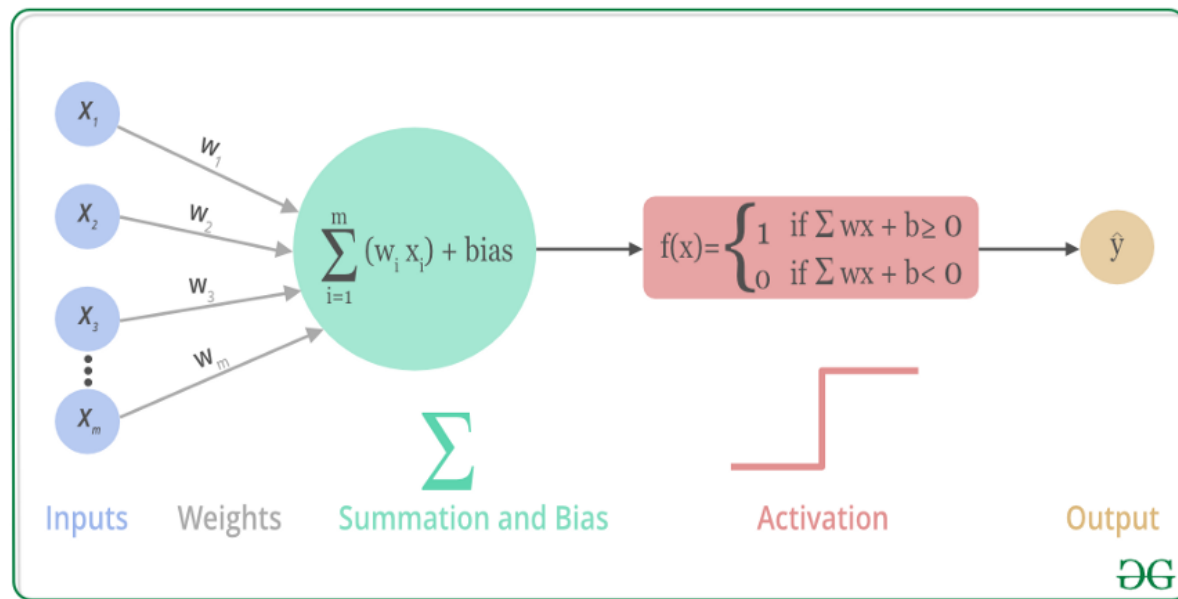
- Training: millions of iterations of forward pass + back propagation to adjust model params (e.g., NN weights); requires large CPU/GPU clusters and days/weeks of training time
- Inference (also called prediction): a single forward pass; can be run on edge devices



```
def train(train_images, train_labels):  
    # build a model for images -> labels...  
    return model  
  
def predict(model, test_images):  
    # predict test_labels using the model...  
    return test_labels
```

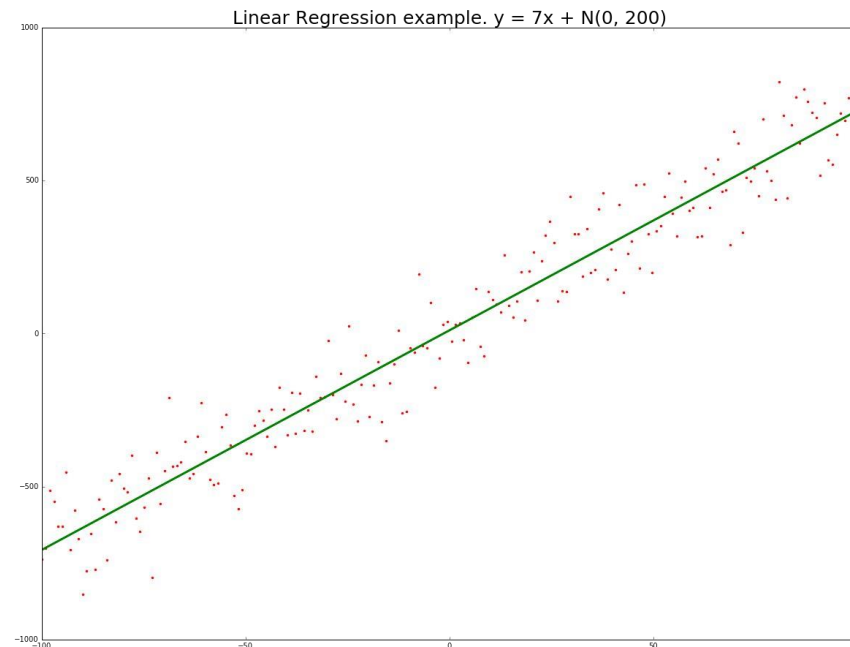
# A Neuron and its Activation Function

- The activation function is a nonlinear monotonic function that acts like a “gate”: the output is larger for larger input activation
  - Perceptron  $y = \sigma(z) = \text{step}(wx + b)$  (activation function  $f =$  step function, shown below)
  - Linear Regression if  $y = z = wx + b$  (activation function  $f =$  identity function)
  - Logistic Regression if  $y = \sigma(z) = \sigma(wx + b)$  (activation function  $f =$  sigmoid function)



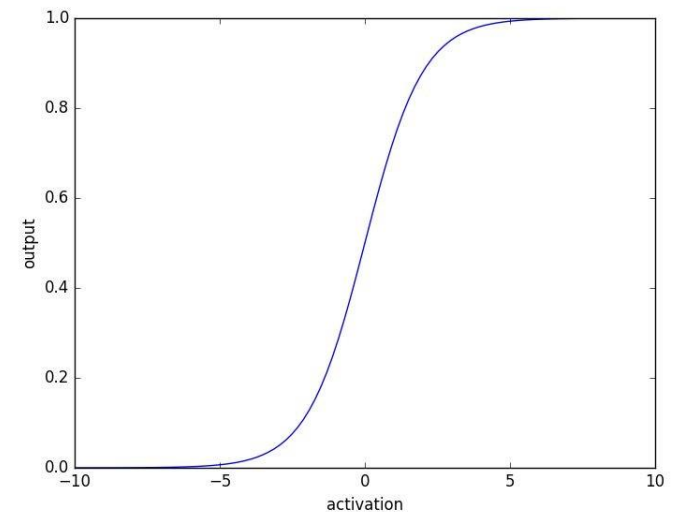
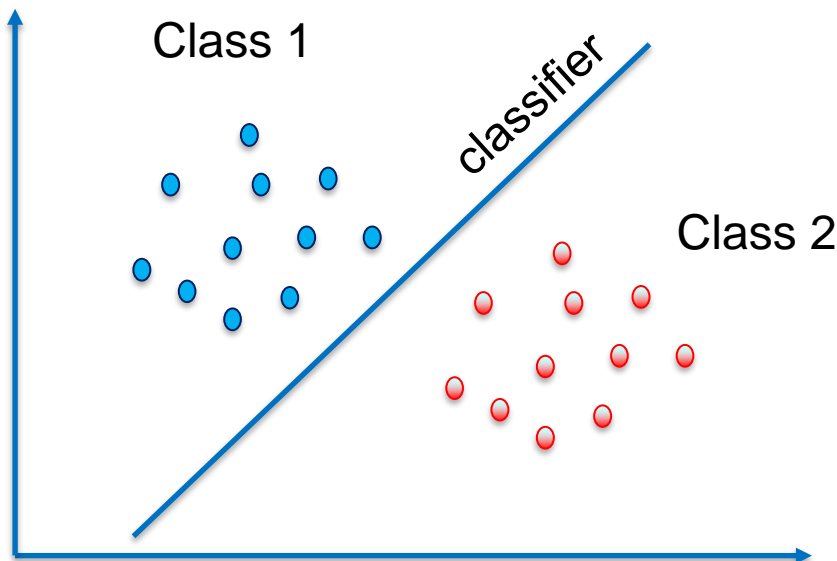
# Linear Regression for Regression

- Function approximation  $y = wx + b$ , with learnable parameters  $\theta = \{w, b\}$ , where  $x, y, b$  are vectors, and  $w$  is a weight matrix
  - e.g., we want to predict price of a house based on its feature vector  $\mathbf{x} = [x_1 \ x_2 \ x_3]^T$ , where  $x_1$  is area in square meters (sqm),  $x_2$  is location ranking (loc),  $x_3$  is year of construction (yoc)
  - Predicted price  $y = wx + b = w_1x_1 + w_2x_2 + w_3x_3 + b$
  - Fig shows an example for scalar  $x$  and  $y$



# Logistic Regression for Binary Classification

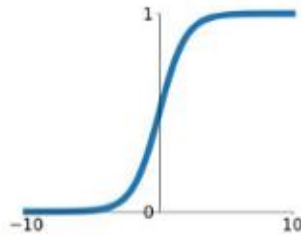
- Consider a binary classification problem: an input image  $x$  may be classified as a dog with probability  $P(y = dog|x)$ , a cat with probability  $P(y = cat|x)$ , with  $P(y = dog|x) + P(y = cat|x) = 1.0$
- Logistic Regression: use sigmoid function  $\sigma(z_i) = \frac{1}{1+e^{-z_i}}$  to map from the activation (also called the logit) to the output probability
- In addition to binary classification at the output layer, sigmoid may also be used as the non-linear activation function in the hidden layers of a NN



# Common Activation Functions used in DL

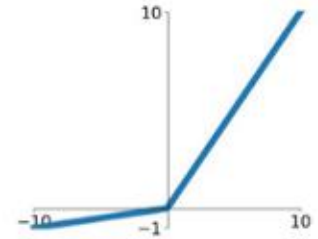
## Sigmoid

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



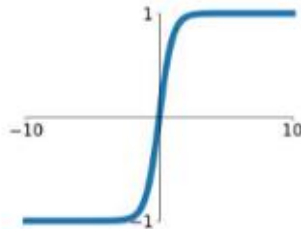
## Leaky ReLU

$$\max(0.1x, x)$$



## tanh

$$\tanh(x)$$

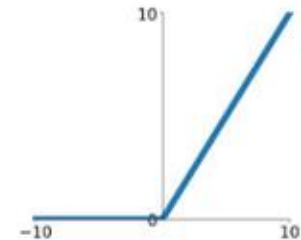


## Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

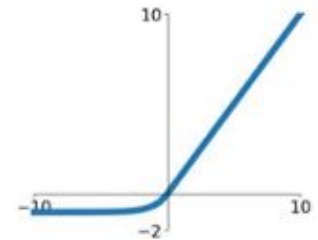
## ReLU

$$\max(0, x)$$



## ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



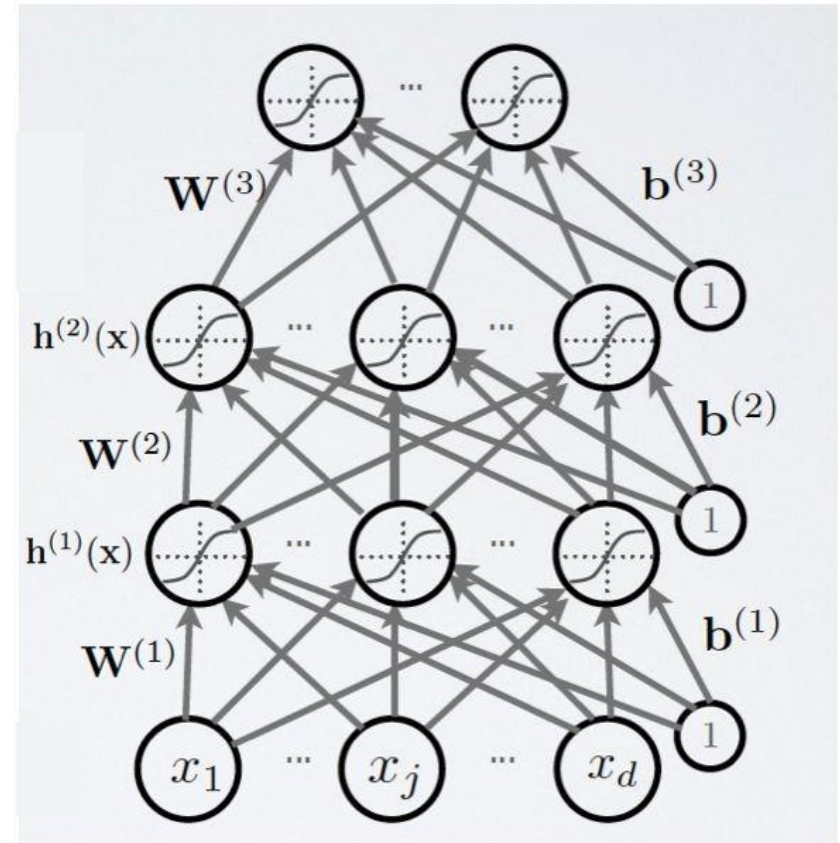


# Deep Neural Networks

- We can stack many hidden layers to form a DNN if we have enough data and computing power to train it
- The high model capacity of DNN comes from non-linear mappings: hidden units must be followed by a non-linear activation function
  - Without non-linear activation functions, a DNN with many layers can be collapsed into an equivalent single-layer NN

# Fully-Connected NNs

- Number of params to learn at i-th layer is  $(N_{i-1} + 1) * N_i$ , where  $N_i$  is the number of neurons at the i-th layer. Can grow very large
  - (We will discuss CNNs with much fewer params in the next lecture)

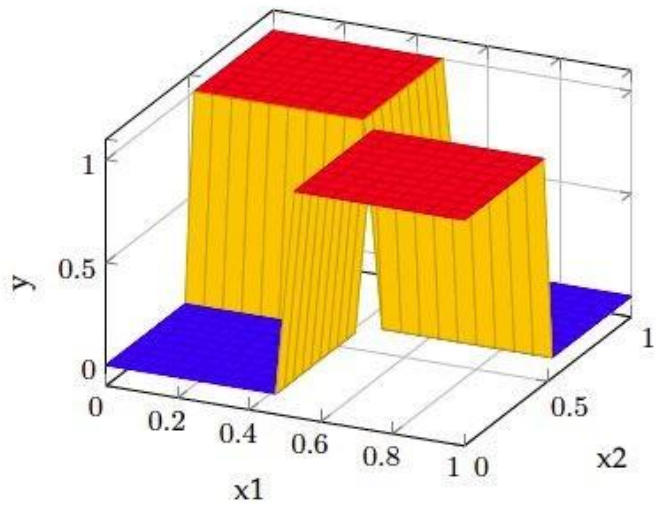


Slide Credit: Hugo Laroché NN course

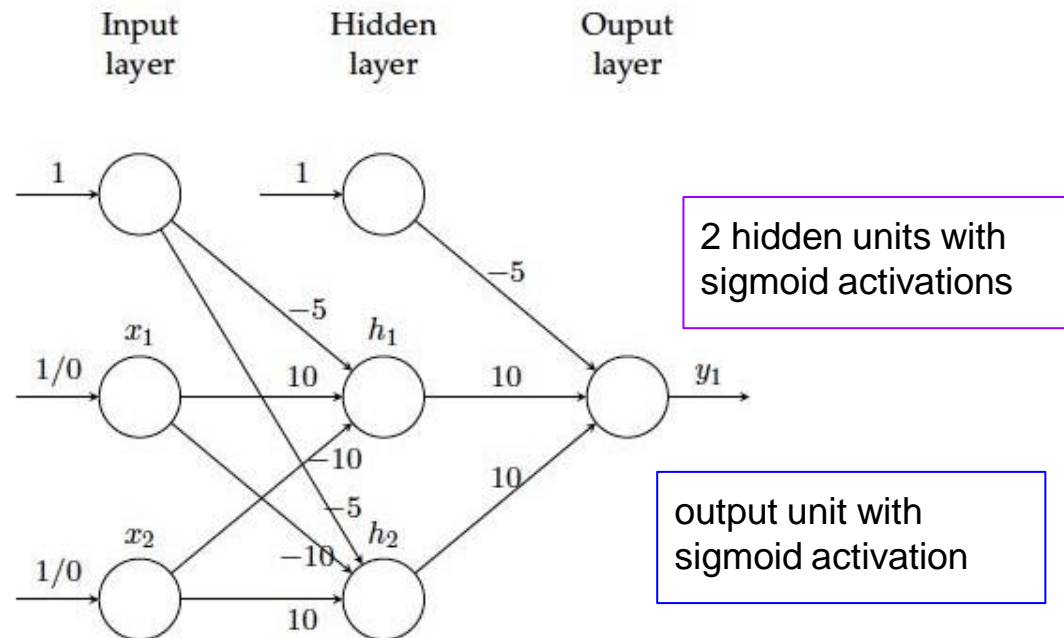
A 3-layer NN

# Example: Two-Layer Fully-Connected NN for Solving XOR

- The NN consists of one input, one hidden, and one output layer, with sigmoid activations

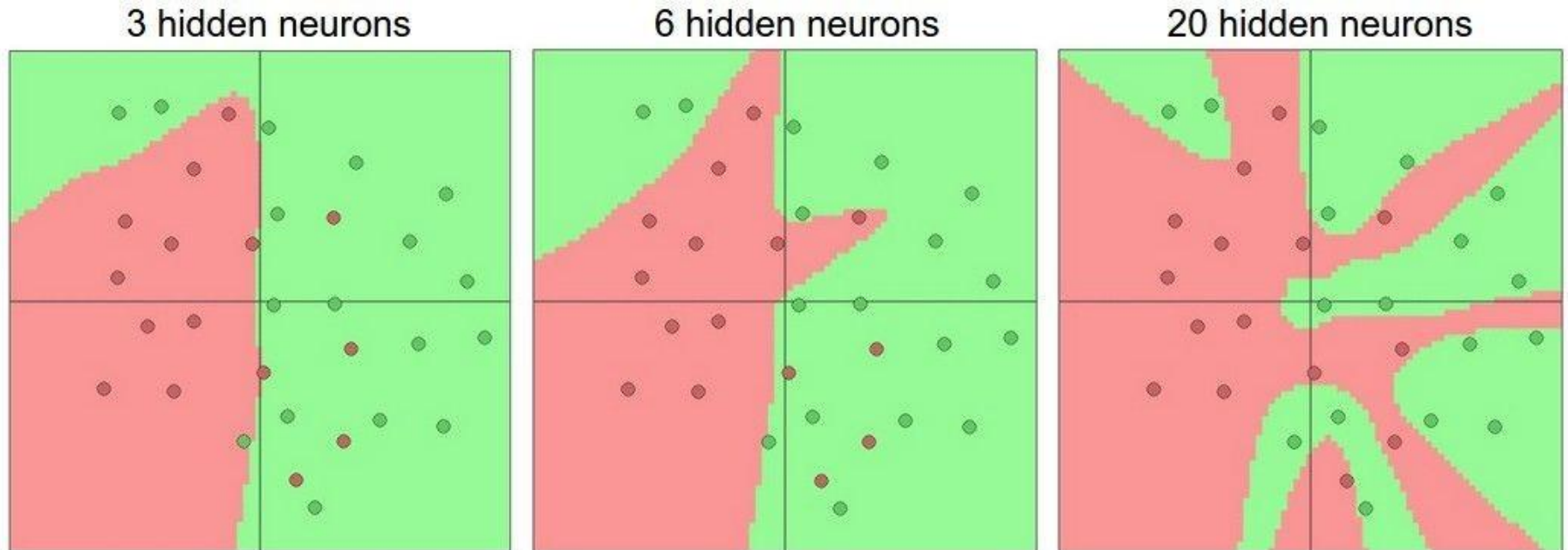


$x_1$	$x_2$	$y$
0	0	0
0	1	1
1	0	1
1	1	0



# Setting # Layers and Their Sizes

- An example illustrating adding more hidden neurons increases model capacity and reduces training error
- But too many layers and neurons may lead to overfitting



# NN for Multi-Class Classification

- Consider a NN defining the model  $h_{\theta}: \mathcal{X} \rightarrow \mathbb{R}^k$ , as the mapping from input  $x$  to output  $h_{\theta}(x)$ , a  $k$ -dim vector of logits, where  $k$  is the number of classes
  - $\theta$  is the set of params (weights and biases)
  - $y$  is the correct label for input  $x$
  - Note that  $h_{\theta}$  does not include the last SoftMax layer
- e.g., a 3-layer NN consisting of 2 layers with ReLU activation functions and a last linear layer is
  - $h_{\theta}(x) = W_3 \max(0, W_2 \max(0, W_1 x + b_1) + b_2) + b_3$



# Cross-Entropy Loss for Multi-Class Classification

- The SoftMax operator  $\sigma: \mathbb{R}^k \rightarrow \mathbb{R}^k$  computes a vector of predicted probabilities  $\sigma(z): \mathbb{R}^k$  from a vector of logits  $z: \mathbb{R}^k$ , where  $k$  is the number of classes:

$$- \sigma(z)_i = \frac{\exp(z_i)}{\sum_{j=1}^k \exp(z_j)}$$

- The loss function is defined as the negative log likelihood of the predicted probability corresponding to the correct label  $y$ :

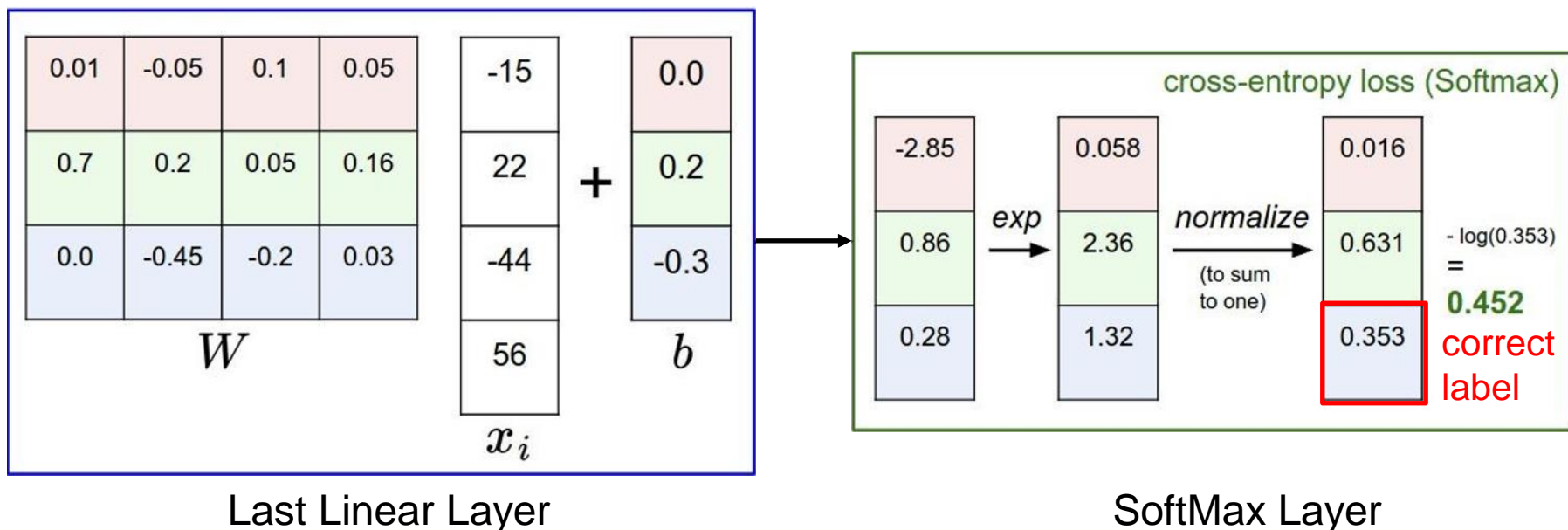
$$- \text{Loss}(h_\theta(x), y) = -\log \sigma(h_\theta(x))_y = -$$

$$\log \left( \frac{\exp(h_\theta(x)_y)}{\sum_{j=1}^k \exp(h_\theta(x)_j)} \right) = \log(\sum_{j=1}^k \exp(h_\theta(x)_j)) - h_\theta(x)_y$$

- Minimizing  $\text{Loss}(h_\theta(x), y)$  amounts to maximizing the logit  $(h_\theta(x))_y$  corresponding to the correct label  $y$

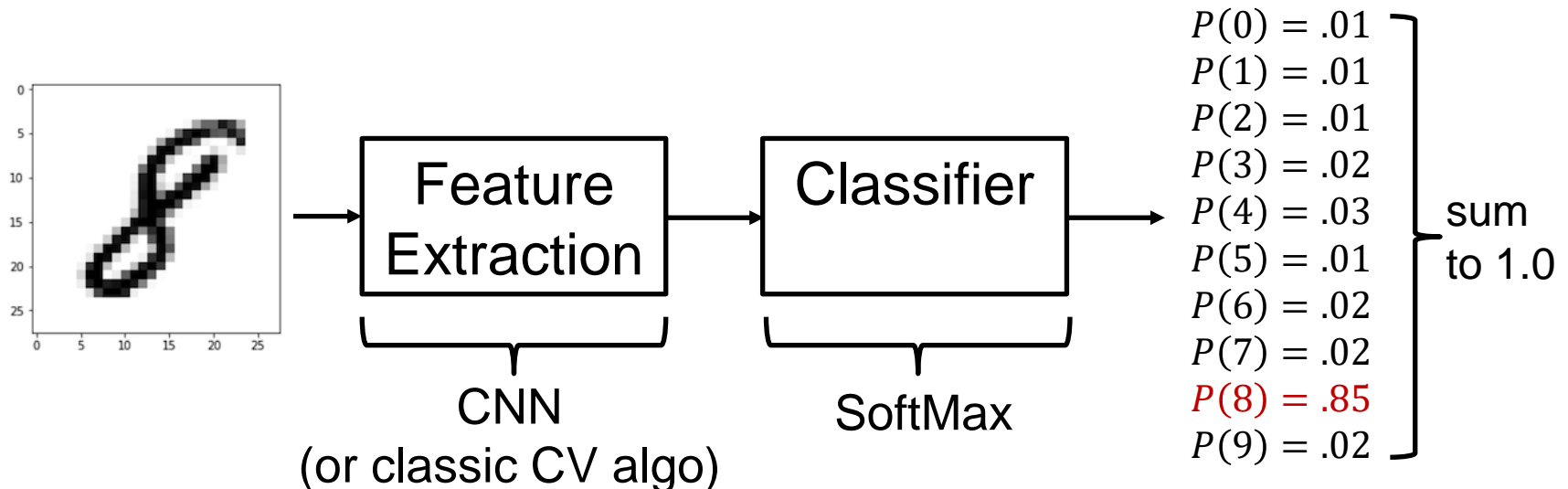
# Cross-Entropy Loss Example

- Consider a NN for 3-class classification. Fig shows the last linear layer and the SoftMax layer
- The last linear layer computes the vector of logits  $h_{\theta}(x) = Wx_i + b = [-2.85 \quad .86 \quad .28]^T$  ( $x$  is the input image to the NN,  $x_i$  is the intermediate input to the last layer)
- The SoftMax layer computes the vector of predicted probabilities  $[.016 \quad .631 \quad .353]^T$  for labels  $[1 \quad 2 \quad 3]^T$ , and the loss  $-\log .353$ , assuming correct label  $y_i = 3$



# Example CV Task: Multi-Class Image Classification

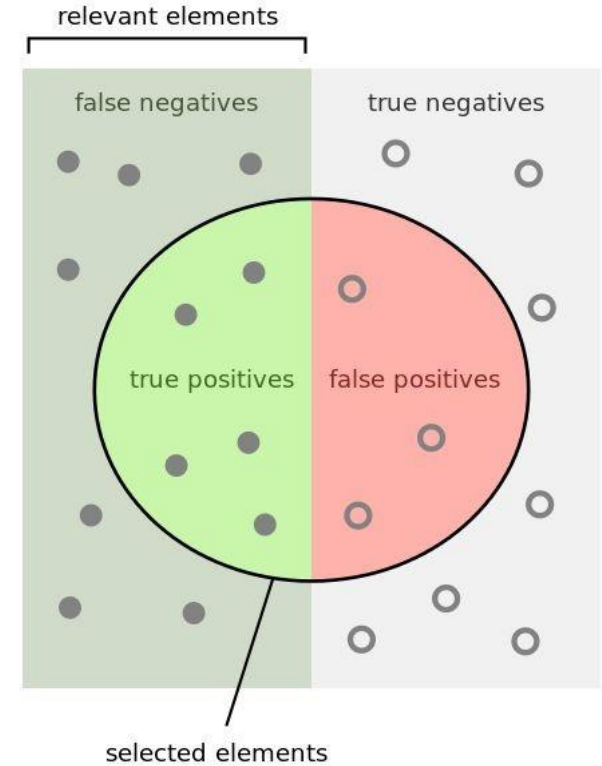
- Two stages: feature extraction from input, and classification based on extracted features
- Classifier returns output as a list of probabilities with size equal to the number of classes, but it may also return the top-1 or top-5 results with highest probability ranking





# Binary Classification Metrics

- The relevant class is considered “positive” in a binary classifier
- e.g., for a medical test that aims to diagnose people with a certain disease. “Positive” denotes sick (has disease), and “negative” denotes healthy (no disease)
  - TP: a sick person is diagnosed as sick
  - TN: a healthy person is diagnosed as healthy
  - FP: a healthy person is misdiagnosed as sick
  - FN: a sick person is misdiagnosed as healthy



How many selected items are relevant?

$$\text{Precision} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Positives}}$$

How many relevant items are selected?

$$\text{Recall} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Negatives}}$$

# Example Confusion Matrix 1

- Precision =  $\frac{TP}{TP+FP} = \frac{100}{100+700} = .125$ 
  - When the classifier predicts positive, it is correct 12.5% of the time
- Recall (TPR) =  $\frac{TP}{TP+FN} = \frac{100}{100+200} \approx .333$ 
  - The classifier catches 33.3% of all the positive cases.
- $F1 = 2 * \frac{\text{Recall} * \text{Precision}}{(\text{Recall} + \text{Precision})} = 2 * \frac{.333 * .125}{.333 + .125} = .182$
- False Positive Rate (FPR) =  $\frac{FP}{FP+TN} = \frac{700}{700+9000} \approx .072$ 
  - The classifier misclassifies 7.2% of the negative cases as positive
- Accuracy =  $\frac{TP+TN}{TP+TN+FP+FN} = \frac{100+9000}{100+9000+700+200} = .91$ 
  - The classifier makes the correct prediction 91% percent of the time
- Positive correlation between TPR vs. FPR; Unpredictable correlation between precision vs. recall

		Predicted / Classified	
		- (Negative)	+ (Positive)
True	- (Negative)	True Negative (TN) 9,000	False Positive (FP) 700
	+ (Positive)	False Negative (FN) 200	True Positive (TP) 100

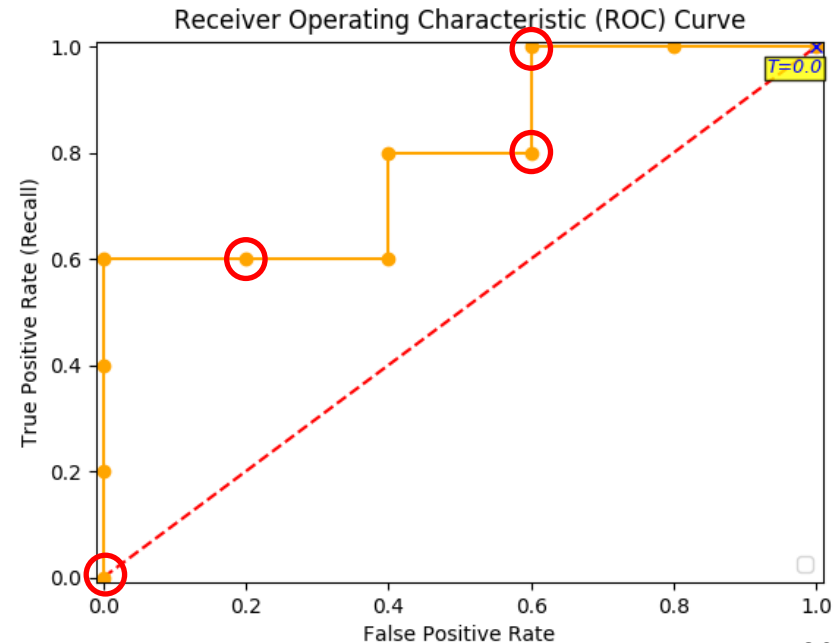
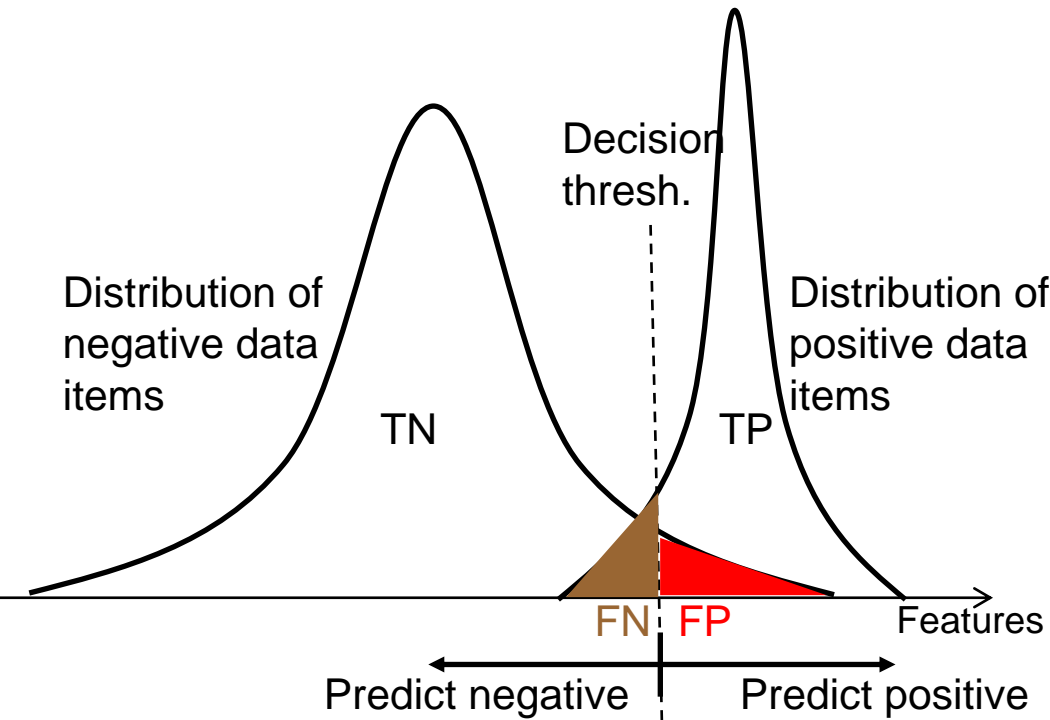
# Example Confusion Matrix 2

- Precision =  $\frac{TP}{TP+FP} = \frac{0}{0+0}$  (ill-defined)
  - When the classifier predicts positive, it is correct ?% of the time (since it never predicts positive, the question is ill-defined)
- Recall (TPR) =  $\frac{TP}{TP+FN} = \frac{0}{0+300} = 0$ 
  - The classifier catches 0% of all the positive cases.
- False Positive Rate (FPR) =  $\frac{FP}{FP+TN} = \frac{0}{0+9700} = 0$ 
  - The classifier misclassifies 0% of the negative cases as positive
- Accuracy =  $\frac{TP+TN}{TP+TN+FP+FN} = \frac{0+9700}{0+9700+0+300} = .97$ 
  - The classifier makes the correct prediction 97% percent of the time
- A medical test that never makes any positive diagnoses is very accurate for a rare disease (diagnose everyone to be healthy), but not very useful

		Predicted / Classified	
		- (Negative)	+ (Positive)
True	- (Negative)	True Negative (TN) 9,700	False Positive (FP) 0
	+ (Positive)	False Negative (FN) 300	True Positive (TP) 0

# ROC and AUC

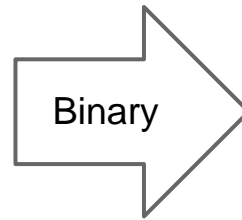
- Binary classification is typically based on a decision threshold parameter. Moving the decision threshold will cause FPR and TPR to move in the same direction
  - e.g., a medical test that sets a lower threshold for positive diagnosis will have both higher FPR and higher TPR, and vice versa
- Receiver Operating Characteristic (ROC) Curve plots FPR (x-axis) vs. TPR (y-axis); Area Under the Curve (AUC) is the area under ROC ( $.5 \leq AUC \leq 1$ , since  $FPR \leq TPR$ )
  - Fig shows an example with 4 points (FPR, TPR) highlighted: (0,0), (.2, .6), (.6, .8), (.6,1.0)
  - The ideal ROC curve:  $FPR \equiv 0, TPR \equiv 1, AUC = 1$ , with  $FP = FN = 0$ ,
  - The worst ROC curve;  $FPR \equiv TPR, AUC = .5$  (dotted line)



# Confusion Matrix for Multi-Class Classification

- Binary classification is a special case of multi-class classification:

$$Accuracy = \frac{\sum_{i=1}^3 x(i, i)}{\sum_{i=1}^3 \sum_{j=1}^3 x(i, j)}$$



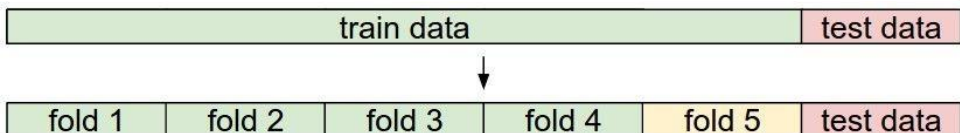
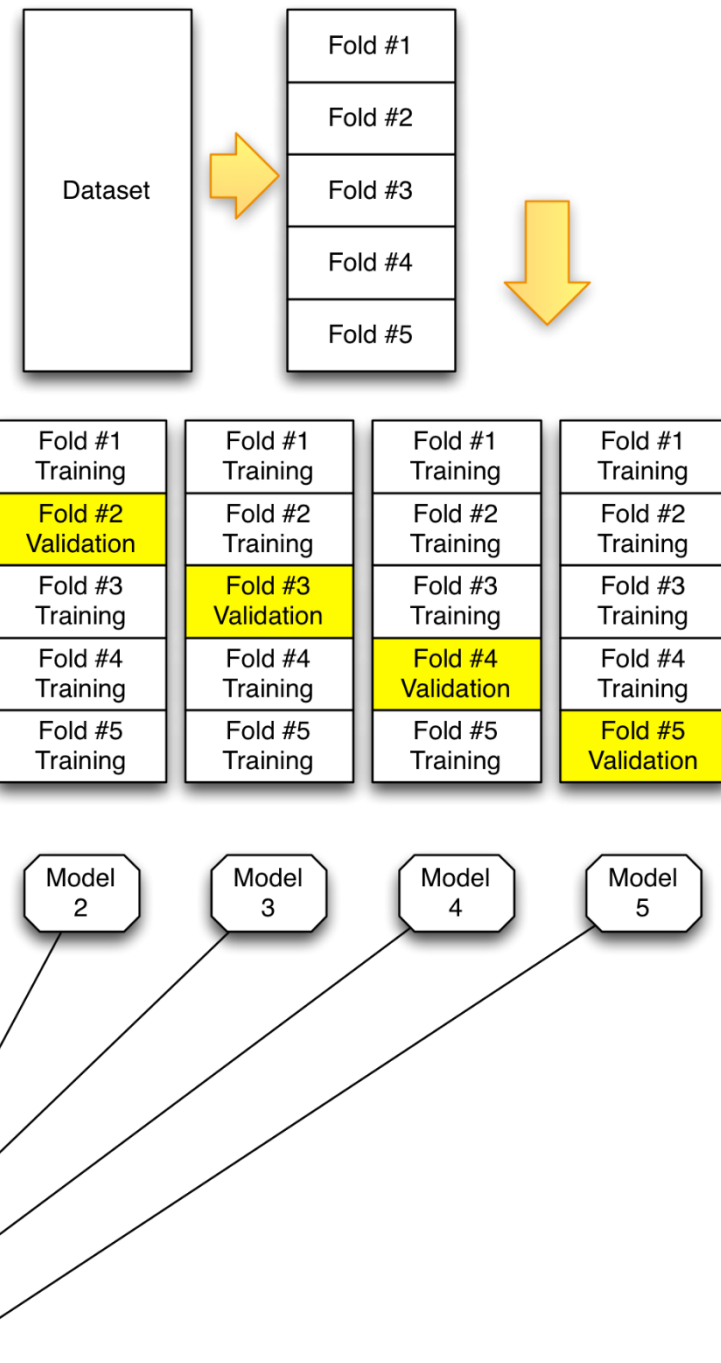
$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

		Prediction		
		Class 1	Class 2	Class 3
Ground Truth	Class 1	x(1,1)	x(1,2)	x(1,3)
	Class 2	x(2,1)	x(2,2)	x(2,3)
	Class 3	x(3,1)	x(3,2)	x(3,3)

		Prediction	
		Positives	negative
Ground Truth	Positives	True positive (TP)	False negative (FN)
	Negative	False positives (FP)	True negative (TN)

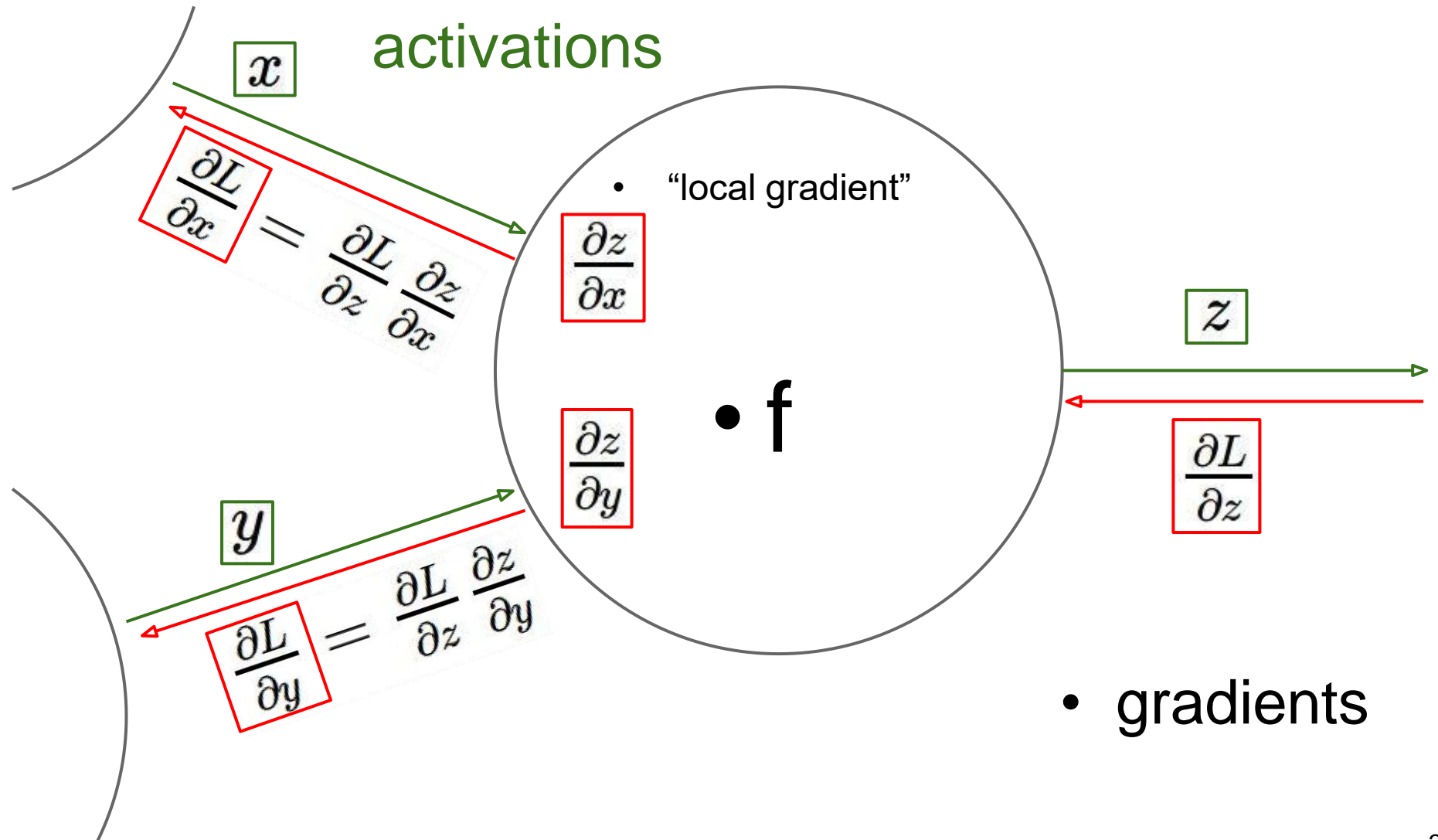
# K-Fold Cross-Validation

- Divide data into train data and test data
- Since we cannot peek at the test data during training time, we use part of the train data for Cross-Validation:
- e.g., Divide training data into  $K=5$  parts (folds). Use each fold as validation data, and the other 4 folds as training data. Cycle through the choice of which fold used for validation and average results.



# Training Neural Networks

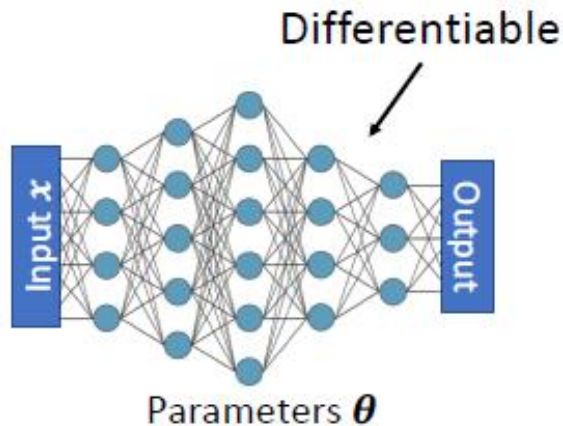
# Local Gradient at One Neuron



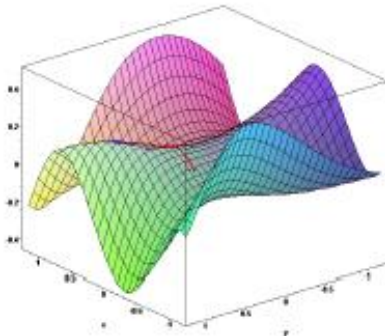


# Gradient Descent

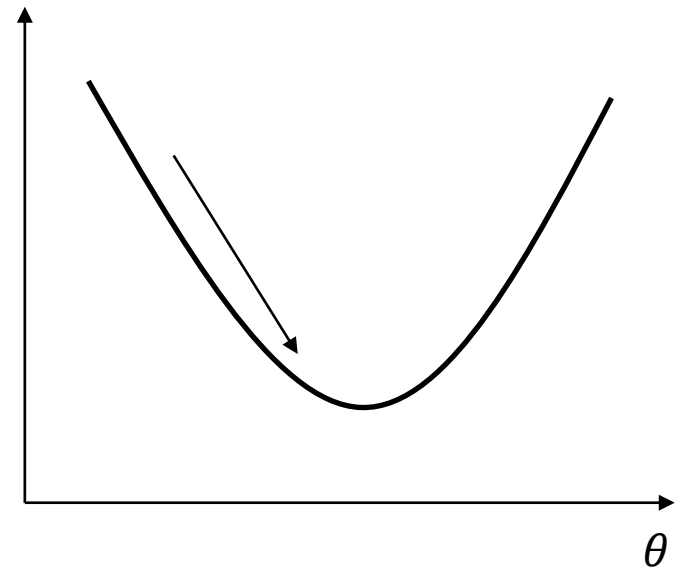
- Gradient descent  $\theta \leftarrow \theta - \alpha \nabla_{\theta} \text{Loss}(x, y; \theta)$
- Loss surface of a DNN is highly non-convex; can only hope to find “reasonably good” local minima



Can use gradient descent method to find good  $\theta$

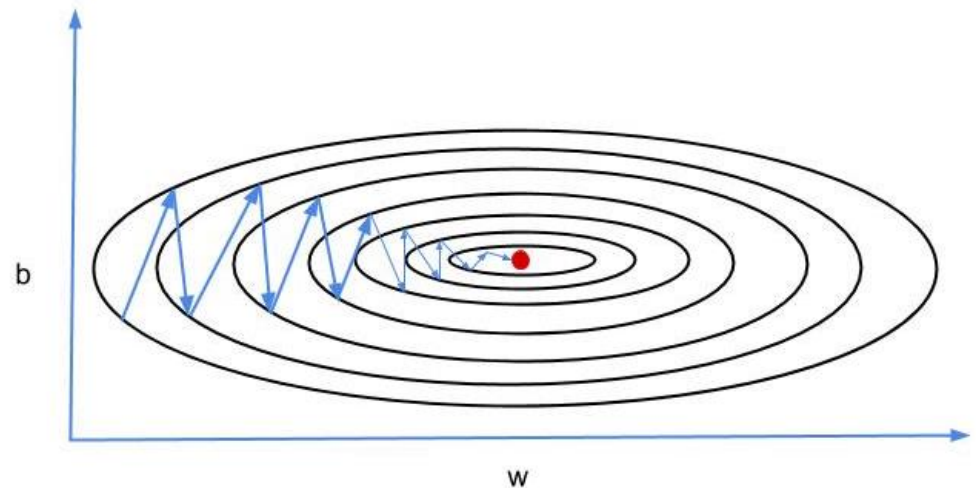
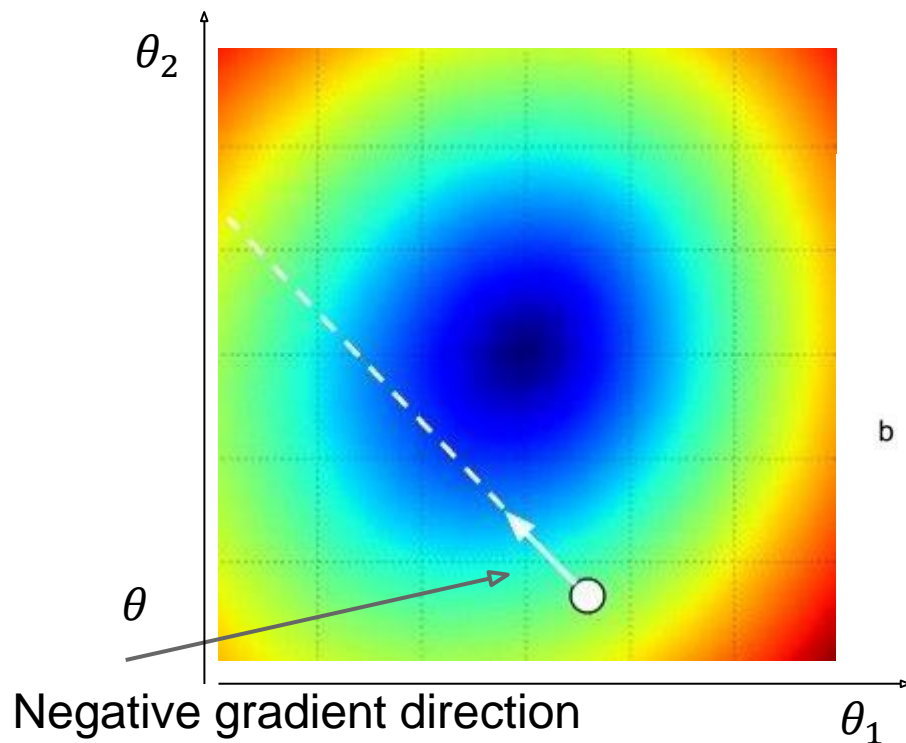


$$\mathbb{E}_{(x,y) \sim D} \text{Loss}(x, y; \theta)$$



# Gradient Descent Algorithms

- Steepest descent may result in in efficient zig-zag path
- More advanced GD methods exploit momentum, e.g., Nesterov, AdaGrad, RMSProp, Adam...



# Mini-batch Stochastic Gradient Descent

- Only use a small portion (a mini-batch) of the training data to compute the gradient
- Common mini-batch sizes are 32/64/128 examples
- Loop:
  - Sample a mini-batch of data
  - Forward prop it through the graph, get loss
  - Backprop to calculate the gradients
  - Update the parameters using gradient descent

# Batch Normalization

- For each mini-batch:
  - 1. Compute the empirical mean and variance independently for each dimension  $i = 1, \dots, m$
  - 2. Normalize to a unit Gaussian with 0 mean and unit variance
- BN layers inserted before nonlinear activation function, and it keeps  $x$ 's average value around 0 for maximum gradient during learning
- Scale and shift params  $\gamma, \beta$  gives more flexibility during training
- Benefits:
  - Improves gradient flow through the network; Allows higher learning rates; Reduces the strong dependence on initialization; Acts as a form of regularization

**Input:** Values of  $x$  over a mini-batch:  $\mathcal{B} = \{x_1, \dots, x_m\}$ ;

Parameters to be learned:  $\gamma, \beta$

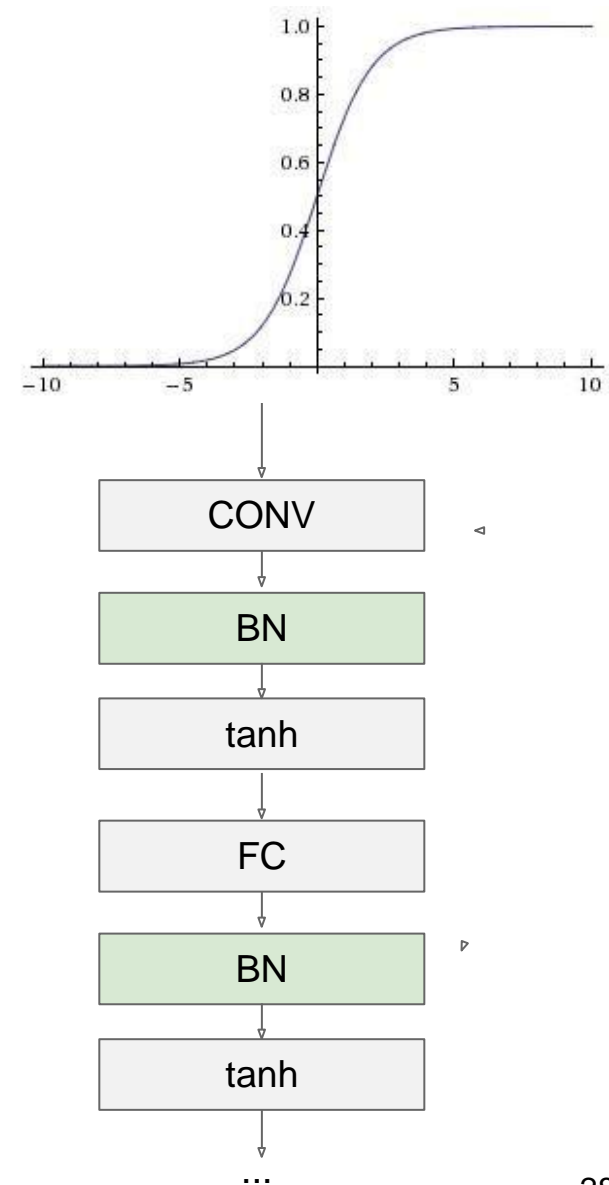
**Output:**  $\{y_i = \text{BN}_{\gamma, \beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^m x_i \quad // \text{ mini-batch mean}$$

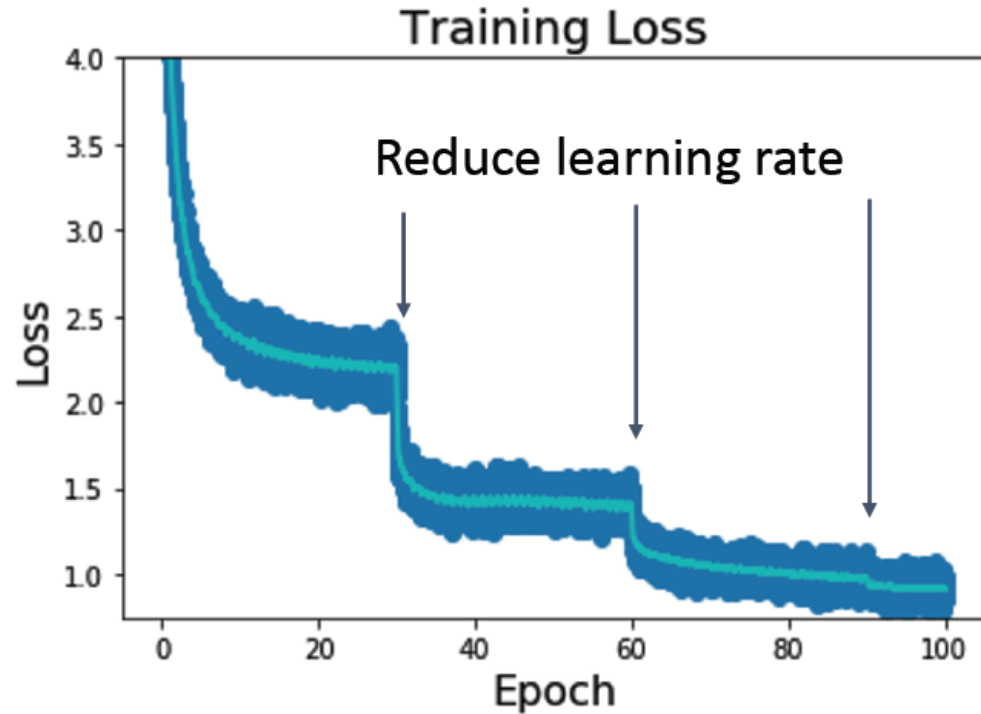
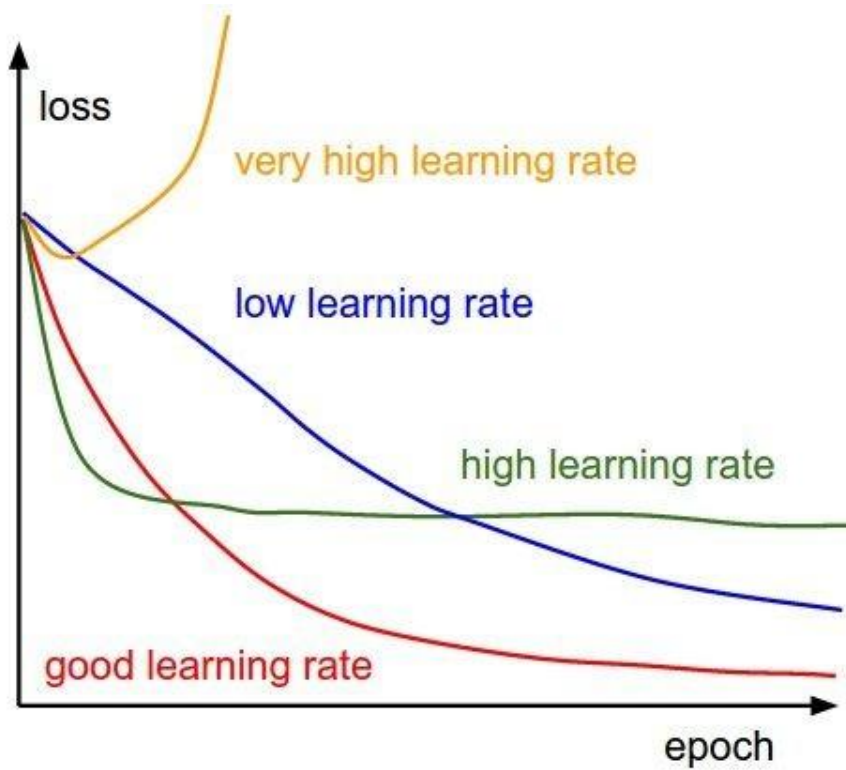
$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2 \quad // \text{ mini-batch variance}$$

$$\hat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \quad // \text{ normalize}$$

$$y_i \leftarrow \gamma \hat{x}_i + \beta \equiv \text{BN}_{\gamma, \beta}(x_i) \quad // \text{ scale and shift}$$

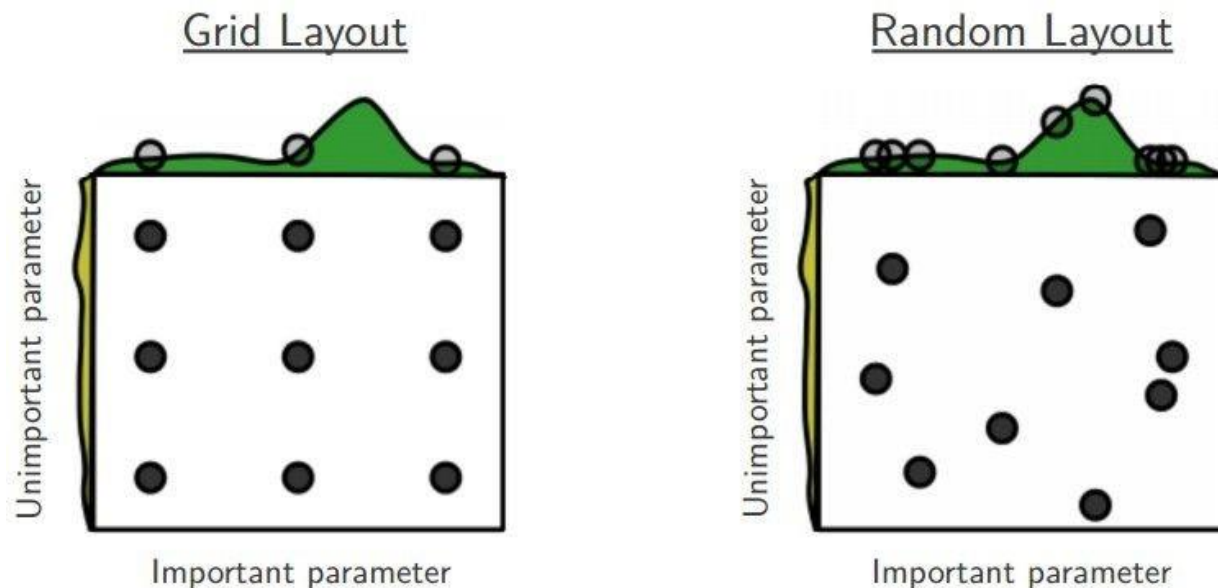


# Learning Rate Schedule during Training



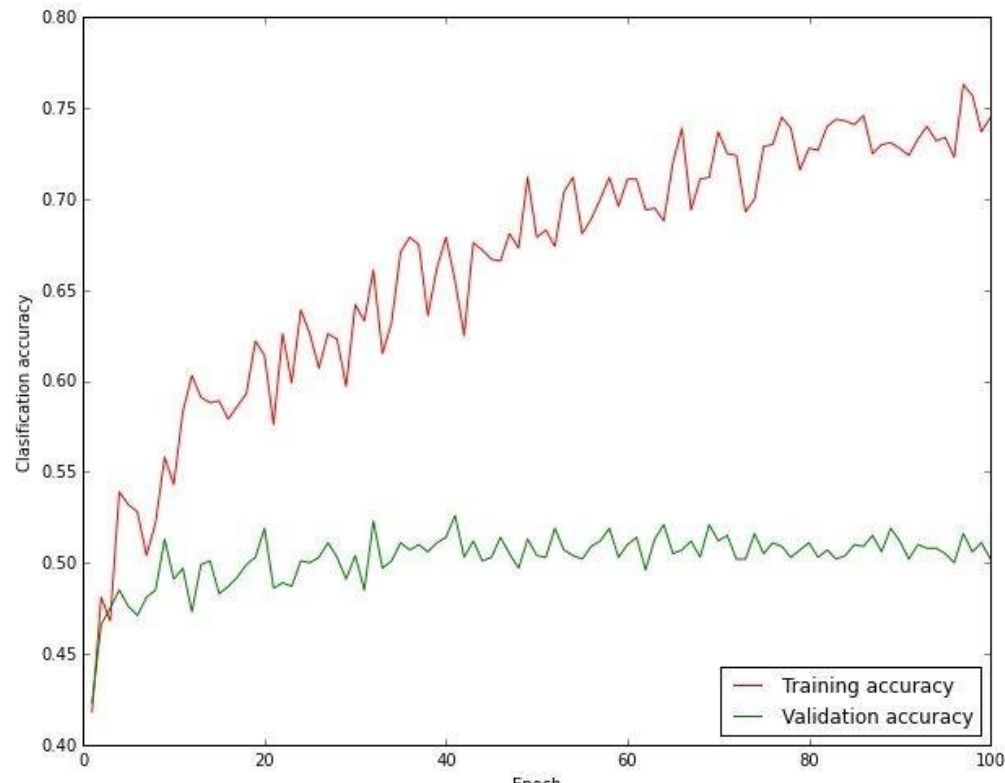
# Hyperparameter Optimization

- Example hyperparams
  - Network architecture
  - Learning rate, its decay schedule, update type
  - Regularization (L2/Dropout strength)
- Grid search vs. random search



# Classification Accuracy

- Big gap between training accuracy and validation accuracy may imply overfitting => decrease model capacity?
- No gap may imply underfitting => increase model capacity?





# Data Augmentation for Enlarging Training Dataset

- Mirroring, random cropping, color shifting, rotation, shearing, local warping...

Mirroring



Random Cropping



Color Shifting

