L2 Introduction to Machine Learning

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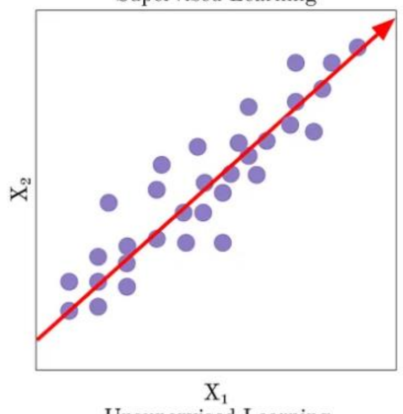
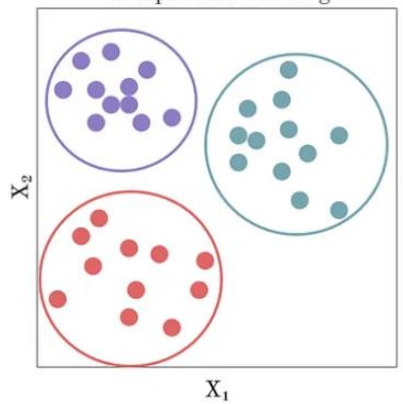
ML Taxonomy

- 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)
- 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.
  - Applications: Game playing (AlphaGo); Robotics; AD…

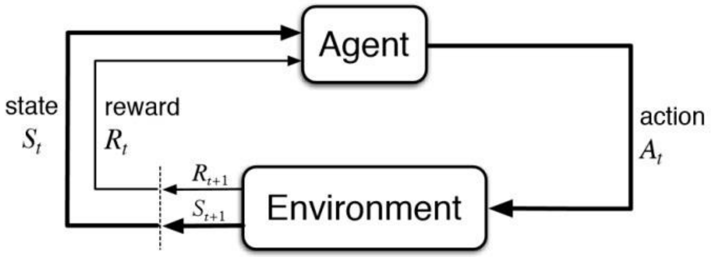
Supervised Learning



Unsupervised Learning

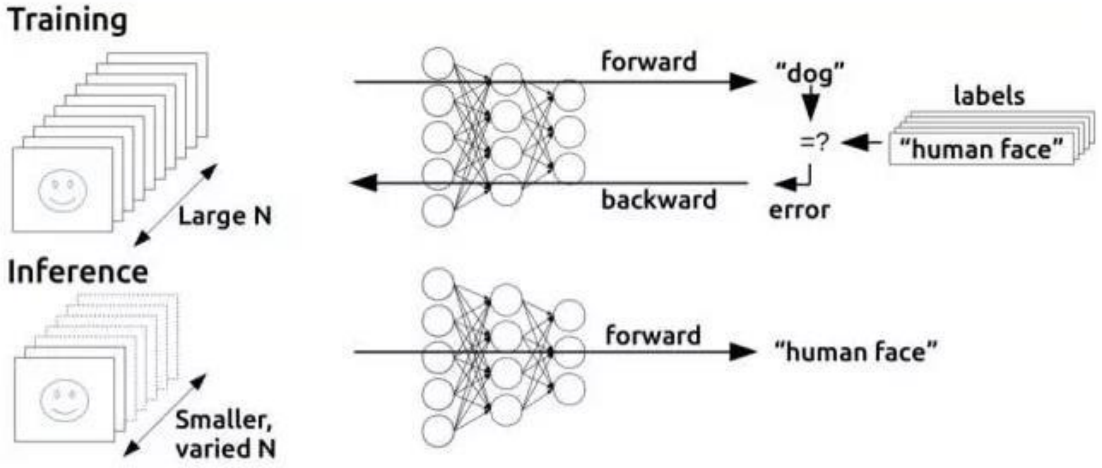


Reinforcement Learning



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

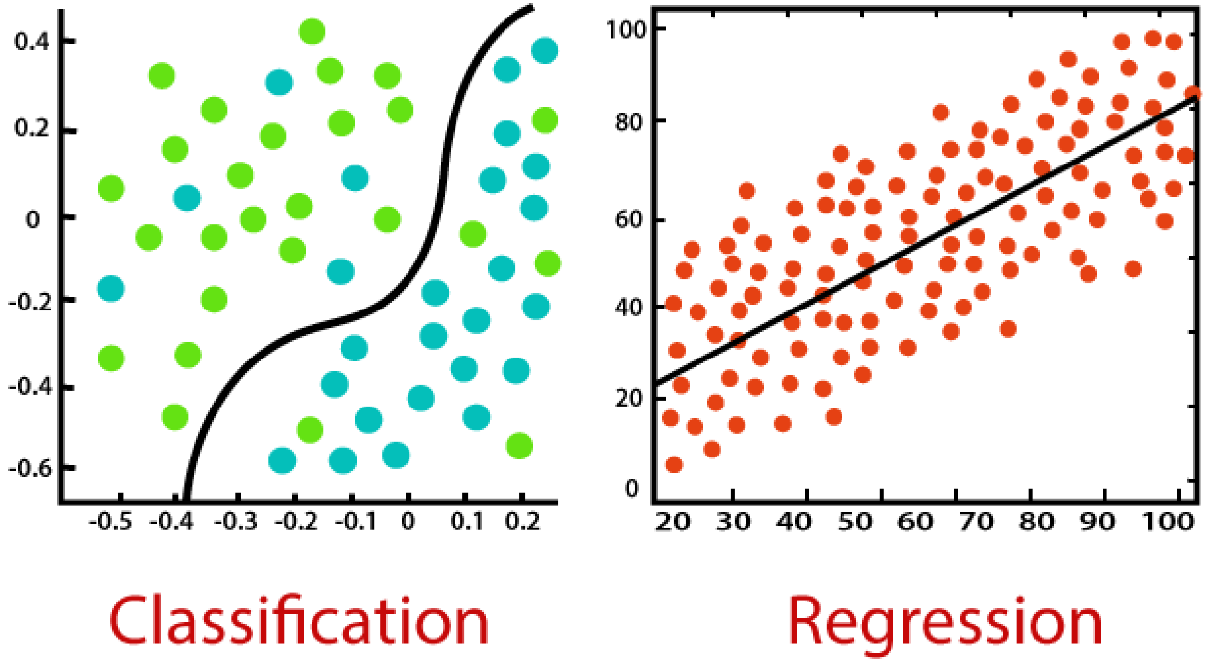



```
def train(train_images, train_labels):
  # build a model for images -> labels...
  return model

def predict(model, test_images):
  # predict test_labels using the model...
  return test_labels
```

Supervised Learning: Classification and Regression

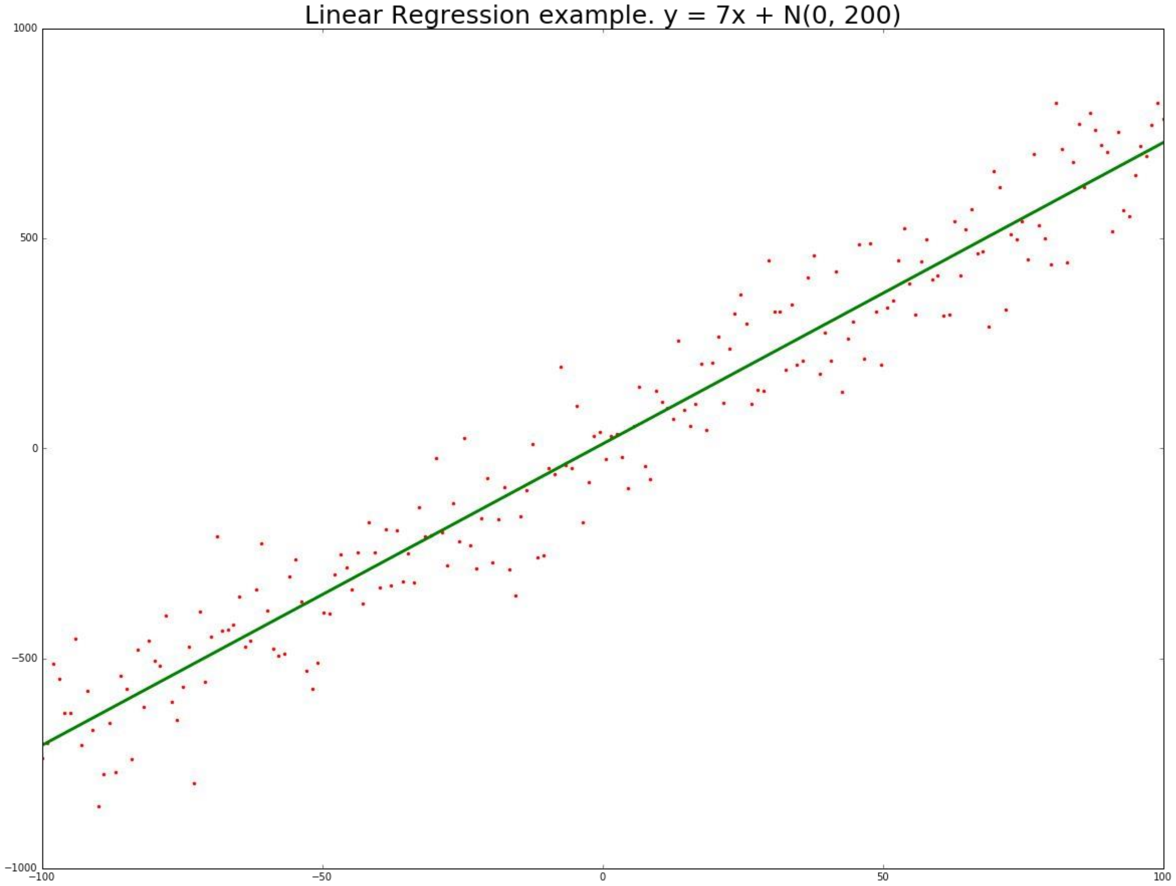
- Both are Supervised Learning algorithms that require ground-truth values as labels.
    - Classification is used to predict/classify discrete labels such as Male or Female, True or False, Spam or Not Spam, etc.
    - Regression is used to predict continuous values such as price, salary, age, etc.
- Loss functions measure how the predicted value differs from ground-truth value.



https://www.javatpoint.com/regression-vs-classification-in-machine-learning

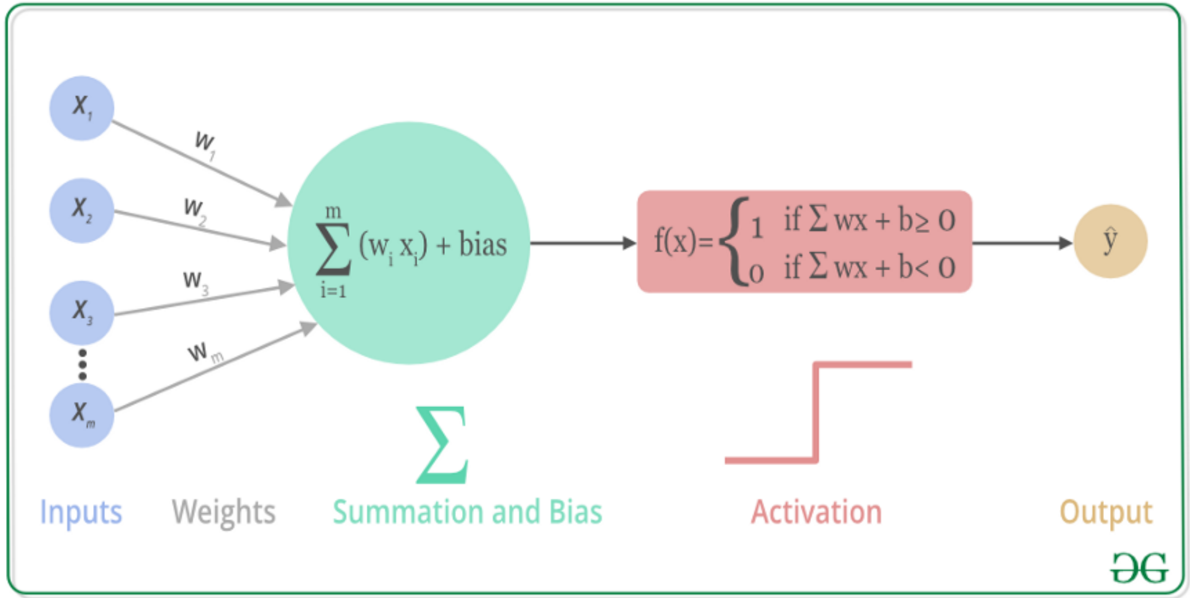
Linear Regression

- 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 $\mathbf{x} = [x_1 \; x_2 \; x_3]^\mathbf{T}$, where x_1 is area in square meters (sqm), x_2 is location ranking (loc), x_3 is year of construction (yoc)
  - Predicted price $y = wx + b = w_1 x_1 + w_2 x_2 + w_3 x_3 + b$
  - Fig shows an example for scalar x and y



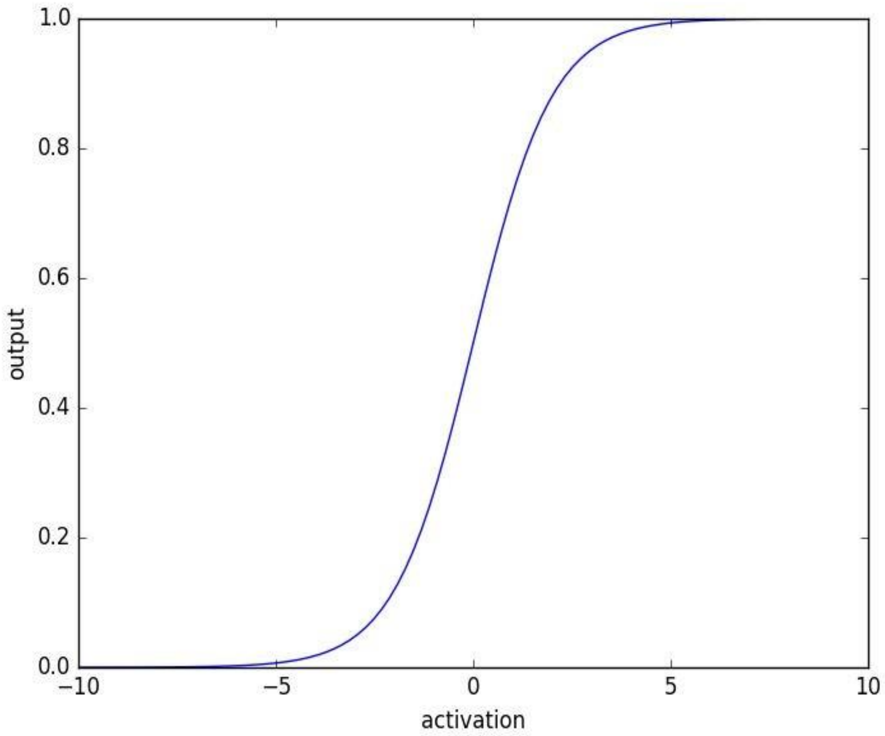
A Neuron and its Activation Function

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



Logistic Regression for Binary Classification

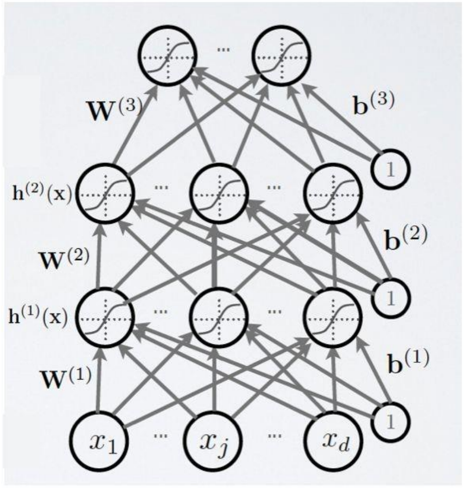
- Consider a binary classification problem: an input image x may be classified as a dog with probability $P(y = dog|x)$, a cat with probability $P(y = cat|x)$, with $P(y = dog|x) + P(y = cat|x) = 1.0$
- Logistic Regression: use sigmoid function $\sigma(z_i) = \frac{1}{1+e^{-z_i}}$ to map from the activation (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



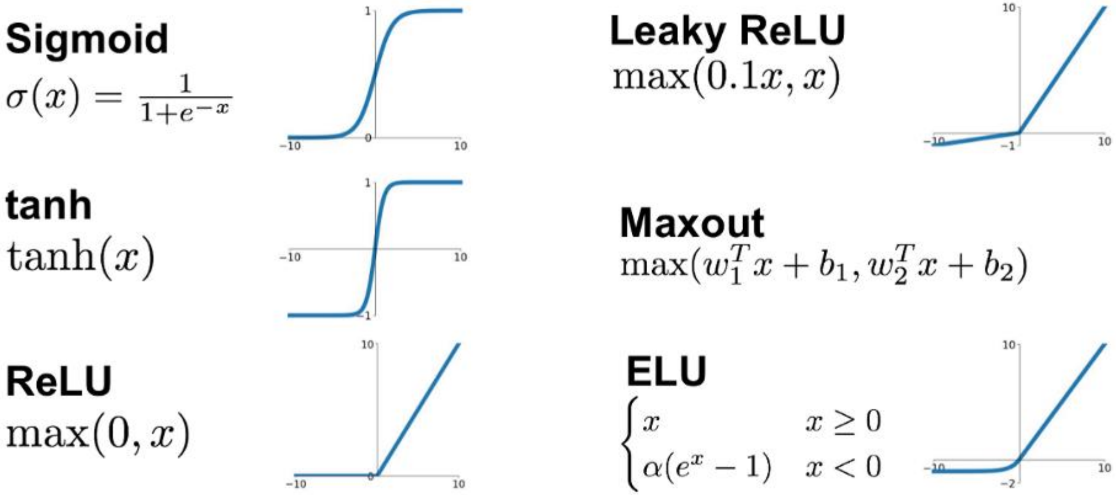
Sigmoid function

Deep Neural Networks and Activation Functions

- 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 activation functions in hidden layers
  - 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 at the 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
  - Convolutional NNs have much fewer params



Slide Credit: Hugo Laroche NN course

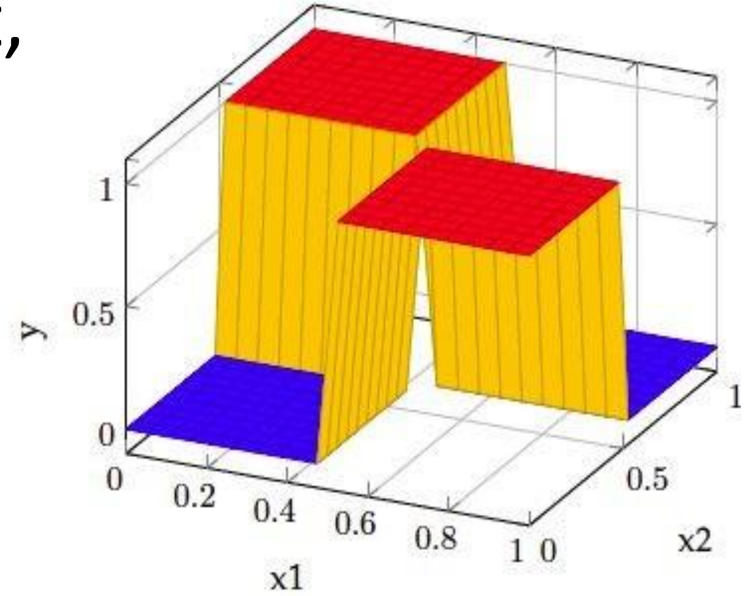


Common Activation Functions

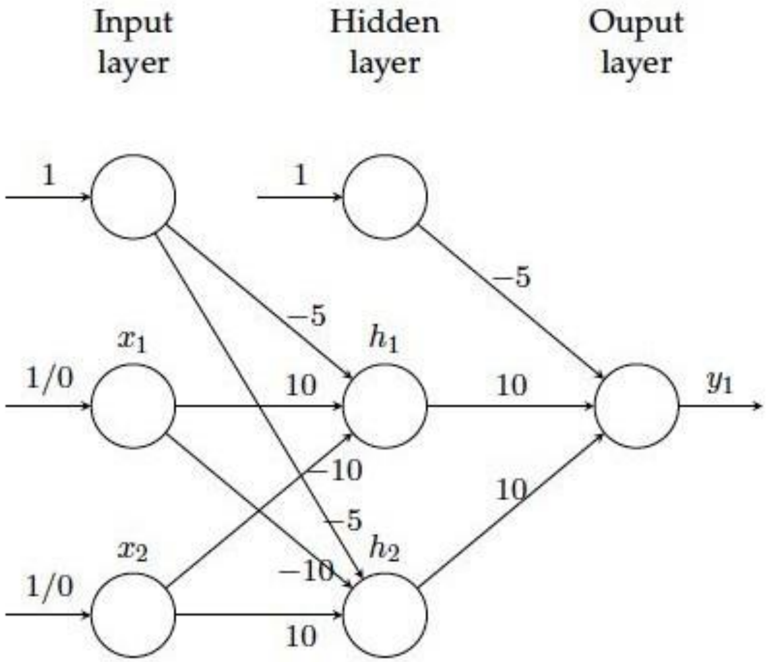
https://laptrinhx.com/complete-guide-of-activation-functions-574622854/

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

- Consists of one input, one hidden, and one output layer, with sigmoid activations

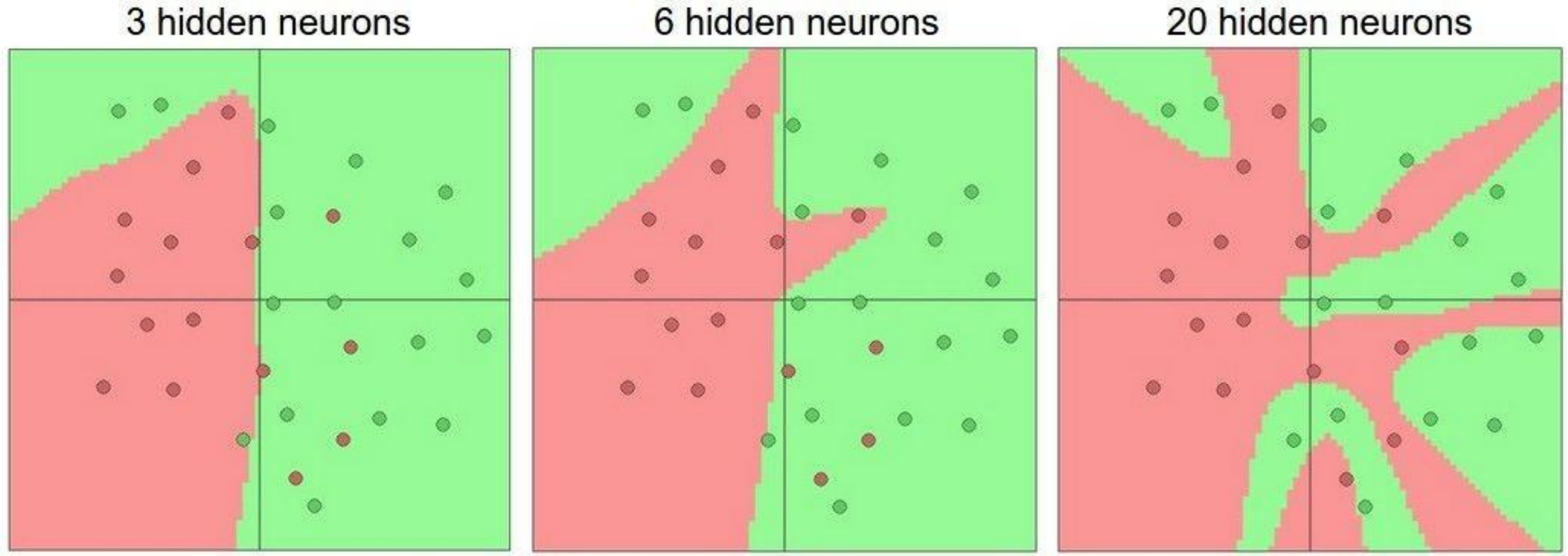


x_1	x_2	y
0	0	0
0	1	1
1	0	1
1	1	0



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



Loss Functions

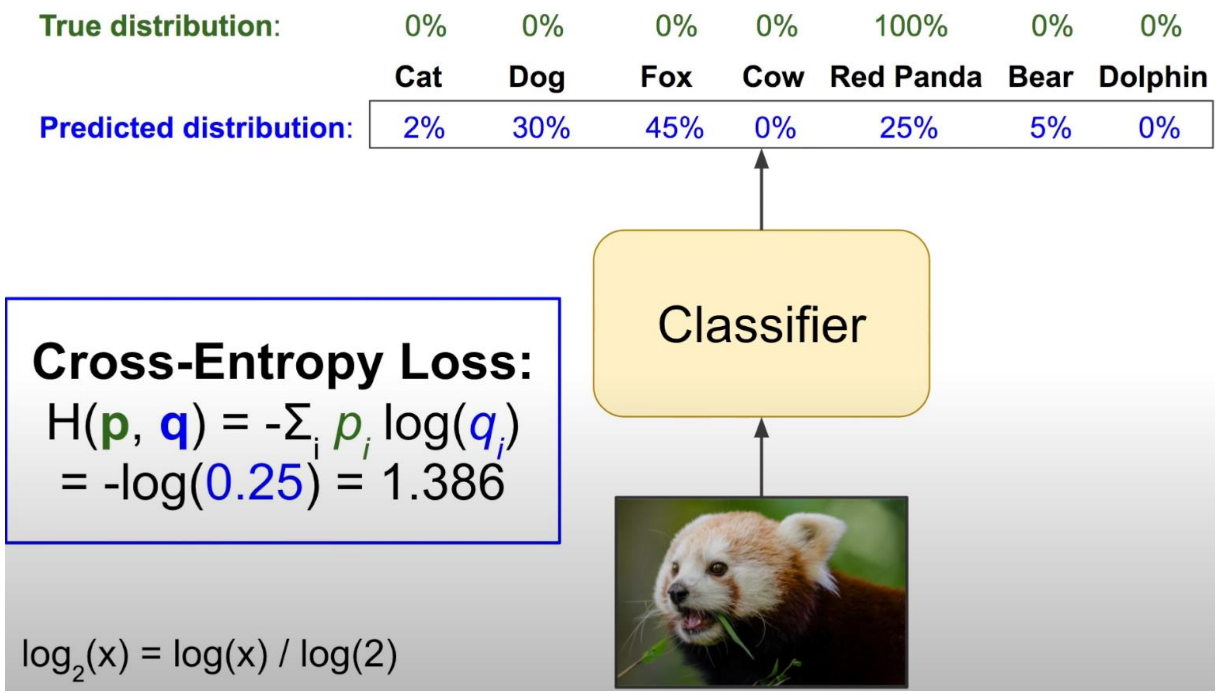
- Classification
  - Cross-Entropy Loss, Log Loss, Focal Loss, Exponential Loss, Hinge Loss…
- Regression
  - MSE (Mean Squared Error)/L2 Loss/Quadratic Loss, MAE (Mean Absolute Error)/L1 Loss, Huber Loss, Log Cosh Loss, Quantile Loss…

NN for Multi-Class Classification

- Consider a NN defining the model $h_\theta: \mathcal{X} \to \mathbb{R}^k$, as the mapping from input x to output $h_\theta(x)$, a k-dim vector of logits, where k is the number of classes
  - θ is the set of params (weights and biases)
  - y is the correct label for input x
  - (Here h_θ does not include the last SoftMax layer that outputs the prediction scores)
- 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

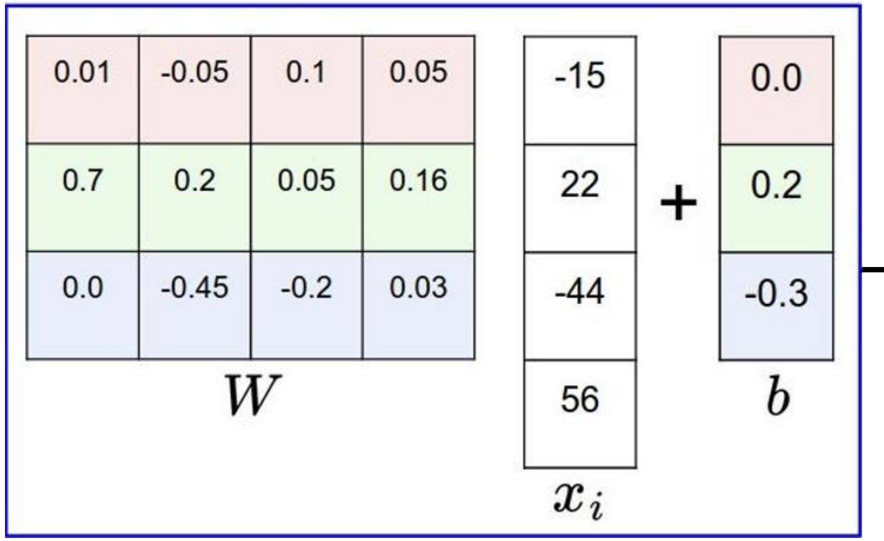
- The SoftMax operator $\sigma: \mathbb{R}^k \to \mathbb{R}^k$ computes a vector of predicted probabilities $\sigma(z): \mathbb{R}^k$ that sum to 1.0, from a vector of logits $z: \mathbb{R}^k$ in the last hidden layer (the penultimate layer), where k is the number of classes:
  - $\sigma(z)_i = \frac{\exp(z_i)}{\sum_{j=1}^{k} \exp(z_j)}$
- The loss function is defined as the negative log likelihood of the predicted probability corresponding to the correct label y:
  - $\text{Loss}(x, y; \theta) = -\log \sigma\left(h_\theta(x)\right)_y = -\log\left(\frac{\exp\left(h_\theta(x)_y\right)}{\sum_{j=1}^{k} \exp\left(h_\theta(x)_j\right)}\right) = \log\left(\sum_{j=1}^{k} \exp\left(h_\theta(x)_j\right)\right) - h_\theta(x)_y$
  - Minimizing $\text{Loss}(h_\theta(x), y)$ amounts to maximizing the logit $\left(h_\theta(x)\right)_y$ corresponding to the correct label y



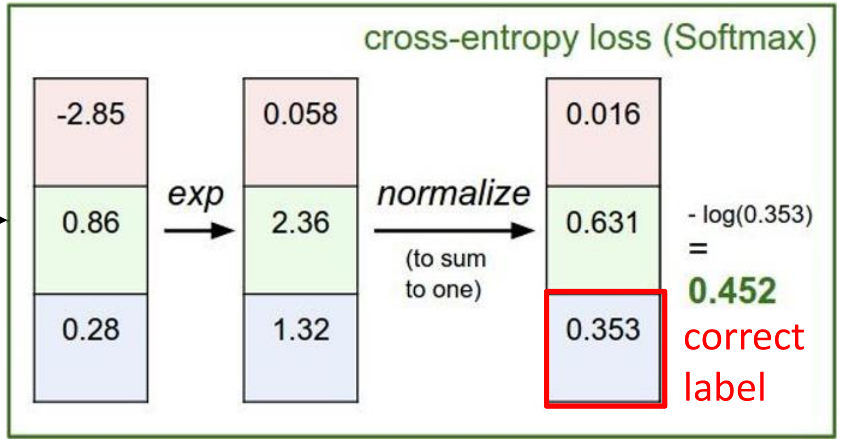
Aurélien Géron A Short Introduction to Entropy, Cross-Entropy and KL-Divergence (YouTube)

CE 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 $y_i = 3$
  - Logits: $[e^{-2.85}, e^{.86}, e^{.28}] = [.058, 2.36, 1.32]$
  - Normalize by $e^{-2.85} + e^{.86} + e^{.28} = 3.738$ to get SoftMax scores $[\frac{.058}{3.738}, \frac{2.36}{3.738}, \frac{1.32}{3.738}] = [.016, .631, .353]$



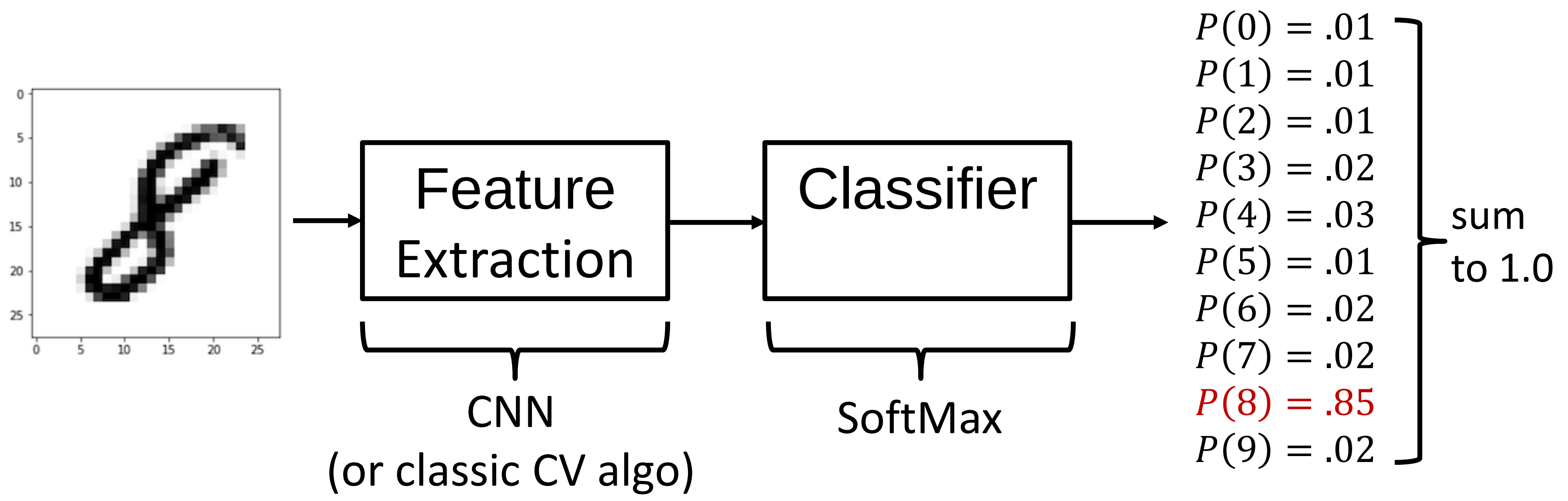
Last Linear Layer



SoftMax Layer

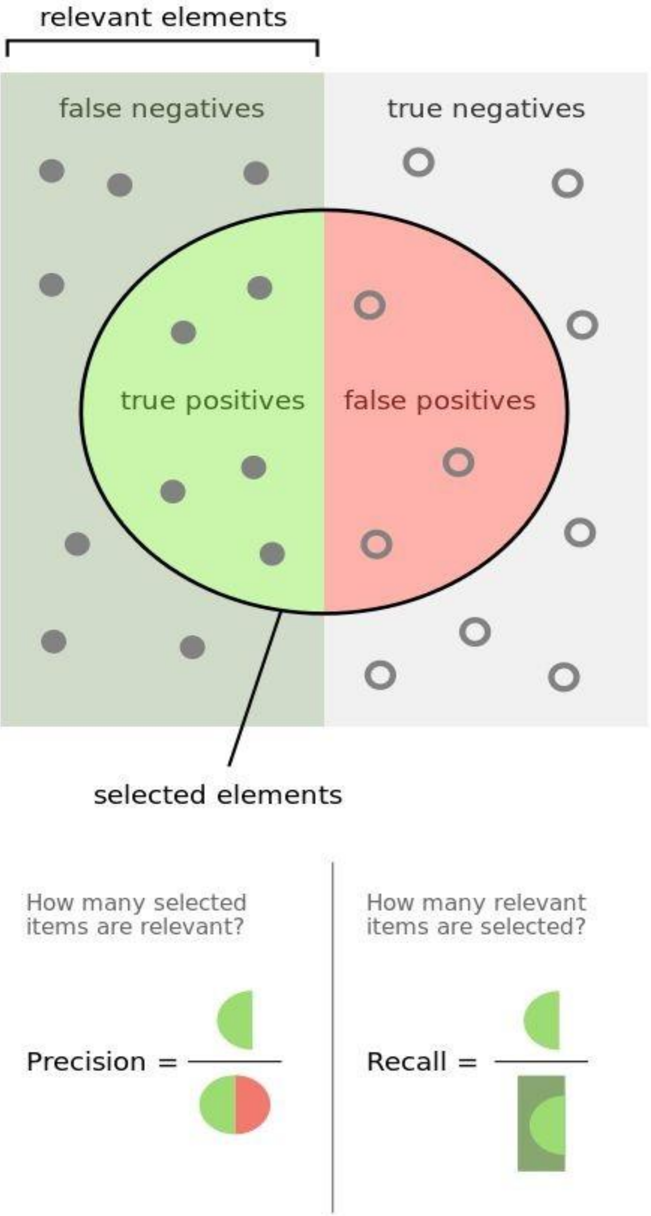
Multi-Class Image Classification

- 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., conswider a medical test that aims to diagnose people with a certain disease. “Positive” denotes sick (has disease), and “Negative” denotes healthy (no disease)
  - True Positive (TP): a sick person is diagnosed as sick
  - True Negative (TN): a healthy person is diagnosed as healthy
  - False Positive (FP): a healthy person is misdiagnosed as sick
  - False Negative (FN): a sick person is misdiagnosed as healthy
- Never Forget Again! // Precision vs Recall with a Clear Example of Precision and Recall by Kimberly Fessel
  - https://www.youtube.com/watch?v=qWfzIYCvBqo



Precision = $\frac{TP}{TP+FP}$, Recall (TPR) = $\frac{TP}{TP+FN}$

Example Confusion Matrix 1

- Precision = $\frac{TP}{TP+FP} = \frac{1}{1+7} = .125$
  - When the classifier predicts positive, it is correct 12.5% of the time
- Recall (True Positive Rate, TPR) = $\frac{TP}{TP+FN} = \frac{1}{1+2} \approx .333$
  - Among all the positive cases, the classier correctly classifies 33.3% of them as positive
- $F1 = 2 * \frac{\text{Precision}*\text{Recall}}{(\text{Precision}+\text{Recall})} = 2 * \frac{.333*.125}{.333+.125} = .182$
- False Positive Rate (FPR) $= \frac{FP}{FP+TN} = \frac{7}{7+90} \approx .072$
  - Among all the negative cases, the classier misclassifies 7.2% of them as positive
- Accuracy = $\frac{TP+TN}{TP+TN+FP+FN} = \frac{1+90}{1+90+7+2} = .91$
  - The classifier makes the correct prediction 91% percent of the time
- Positive correlation between TPR vs. FPR
- In general, negative correlation between precision vs. recall (but not strictly monotonic)

		Ground Truth	
		Positive	Negative
Predicted	Neg	False Negative (FN)=2	True Negative (TN)=90
	Pos	True Positive (TP)=1	False Positive (FP)=7

https://medium.com/swlh/recall-precision-f1-roc-auc-and-everything-542aedf322b9

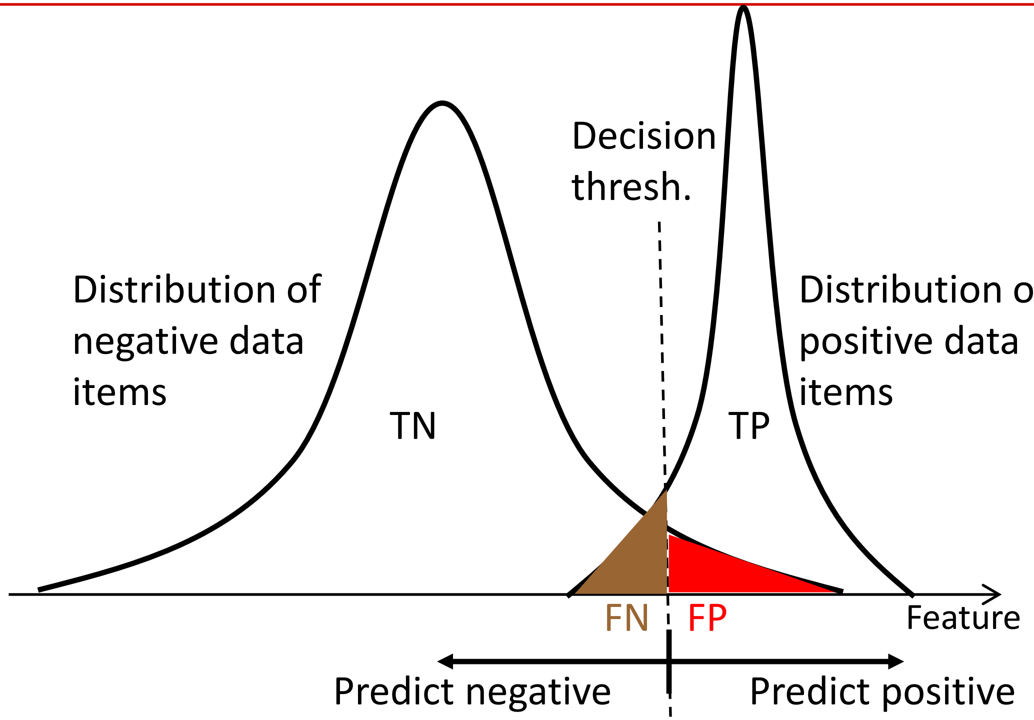
Example Confusion Matrix 2

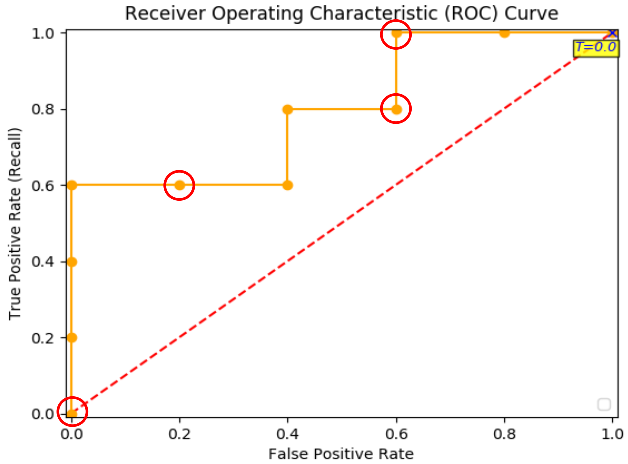
- Precision = $\frac{TP}{TP+FP} = \frac{0}{0+0}$ (ill-defined)
  - When the classifier predicts positive, it is correct ?% of the time (since it never predicts positive, the question is ill-defined)
- Recall (TPR) = $\frac{TP}{TP+FN} = \frac{0}{0+3} = 0$
  - Among all the positive cases, the classier correctly classifies 0% of them as positive
- FPR $= \frac{FP}{FP+TN} = \frac{0}{0+97} = 0$
  - Among all the negative cases, the classier misclassifies 0% of them as positive
- Accuracy = $\frac{TP+TN}{TP+TN+FP+FN} = \frac{0+97}{0+97+0+3} = .97$
  - The classifier makes the correct prediction 97% percent of the time
- A medical test that never makes any positive diagnoses is highly accurate for a rare disease (diagnose everyone to be healthy), but completely useless

		Ground Truth	
		Positive	Negative
Predicted	Neg	False Negative (FN)=3	True Negative (TN)=97
	Pos	True Positive (TP)=0	False Positive (FP)=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
  - Lower threshold for positive prediction leads to 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 ($.5 \leq ROC \leq 1$, 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

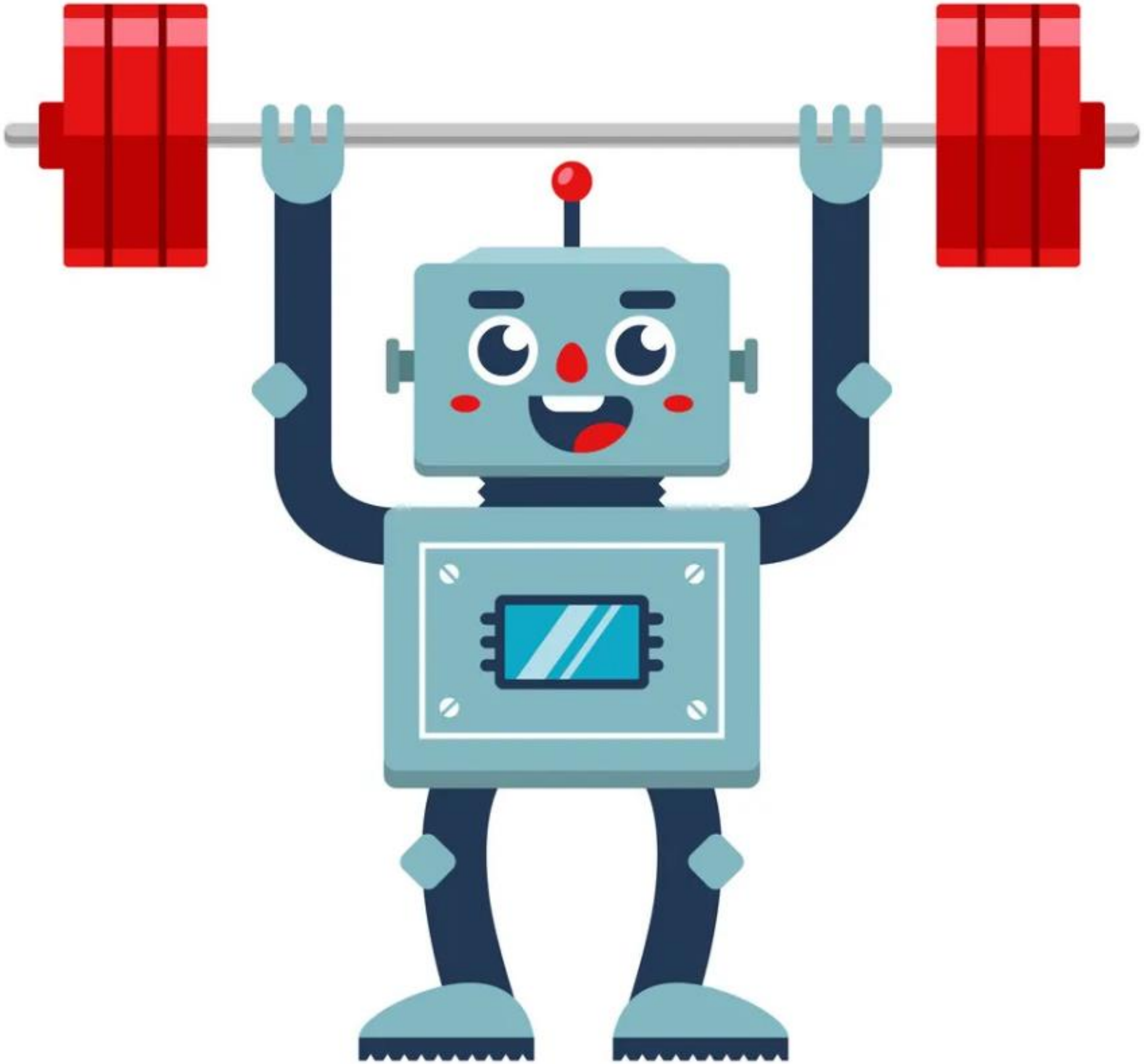
- Binary classification is a special case of multi-class classification

$$Accuracy = \frac{\boxed{\sum_{i=1}^{3} x(i,i)}}{\boxed{\sum_{i=1}^{3}\sum_{j=1}^{3} x(i,j)}} \xrightarrow{\text{Binary}} Accuracy = \frac{\boxed{TP+TN}}{\boxed{TP+TN+FP+FN}}$$

		Ground Truth		
		Cls1	Cls2	Cls3
Pred.	Cls3			
	Cls2			
	Cls1			

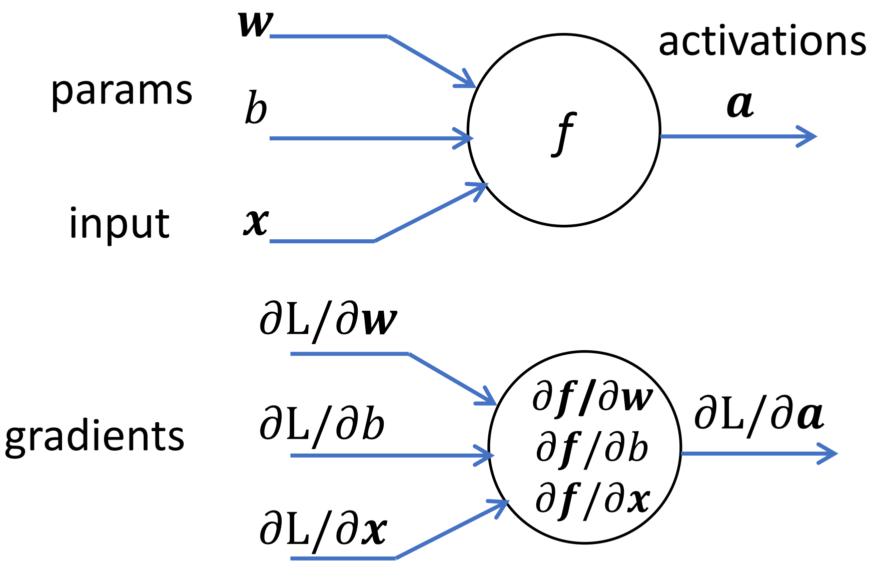
		Ground Truth	
		Pos	Neg
Pred.	Pos	FN	TN
	Neg	TP	FP

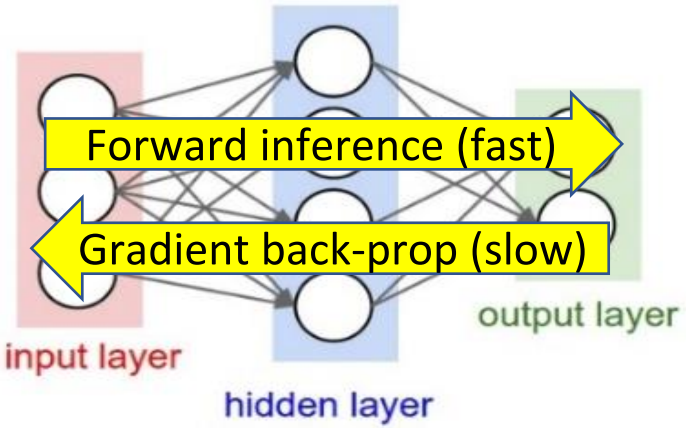
Training Neural Networks



Back-Propagation for NN Training

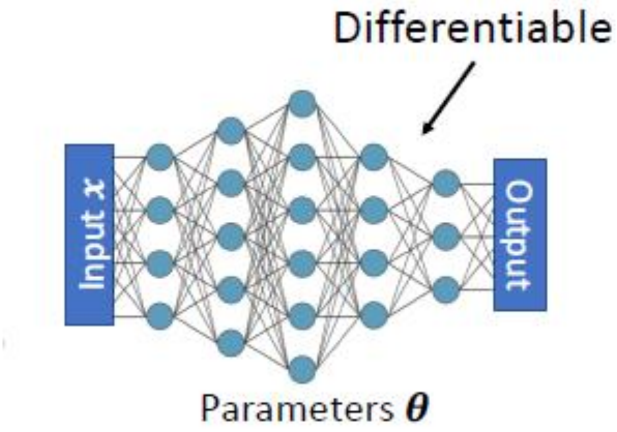
- Consider a single neuron denoted as a function f
- Forward inference: computing its output activation $\boldsymbol{a}$ based on its input $\boldsymbol{x}$, weight $\boldsymbol{w}$, and bias b: $\boldsymbol{a} = \boldsymbol{w}\boldsymbol{x} + b$
- Back-propagation: computing gradients with chain rule, and use gradient descent to update weights and biases:
  - $\frac{\partial \mathrm{L}}{\partial \boldsymbol{w}} = \frac{\partial \mathrm{L}}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{w}}, \frac{\partial \mathrm{L}}{\partial \boldsymbol{b}} = \frac{\partial \mathrm{L}}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{b}}, \frac{\partial \mathrm{L}}{\partial \boldsymbol{x}} = \frac{\partial \mathrm{L}}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}$



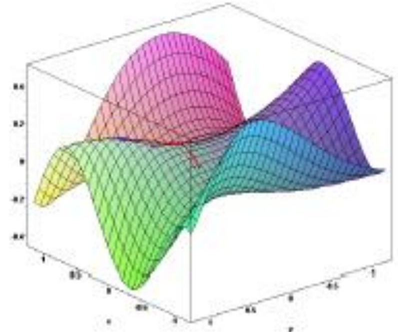


Gradient Descent

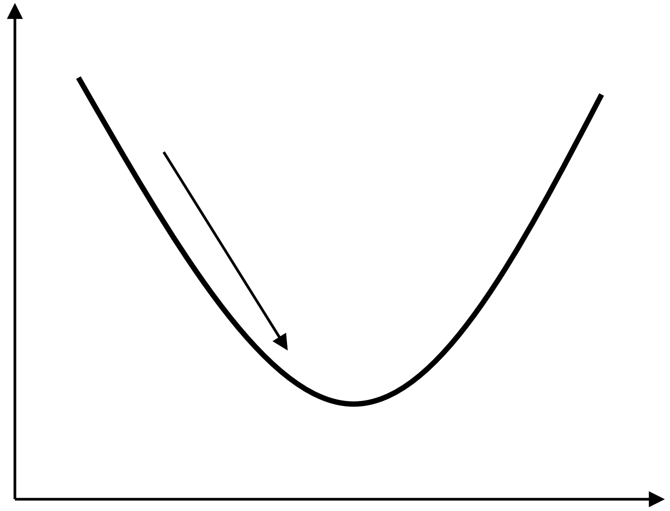
- To minimize the expected loss over training dataset D, use gradient descent $\theta \leftarrow \theta - \alpha\nabla_\theta \mathrm{Loss}(x, y; \theta)$
- Loss surface of a DNN is highly non-convex; can only hope to find “reasonably good” local minima



Can use gradient descent method to find good θ

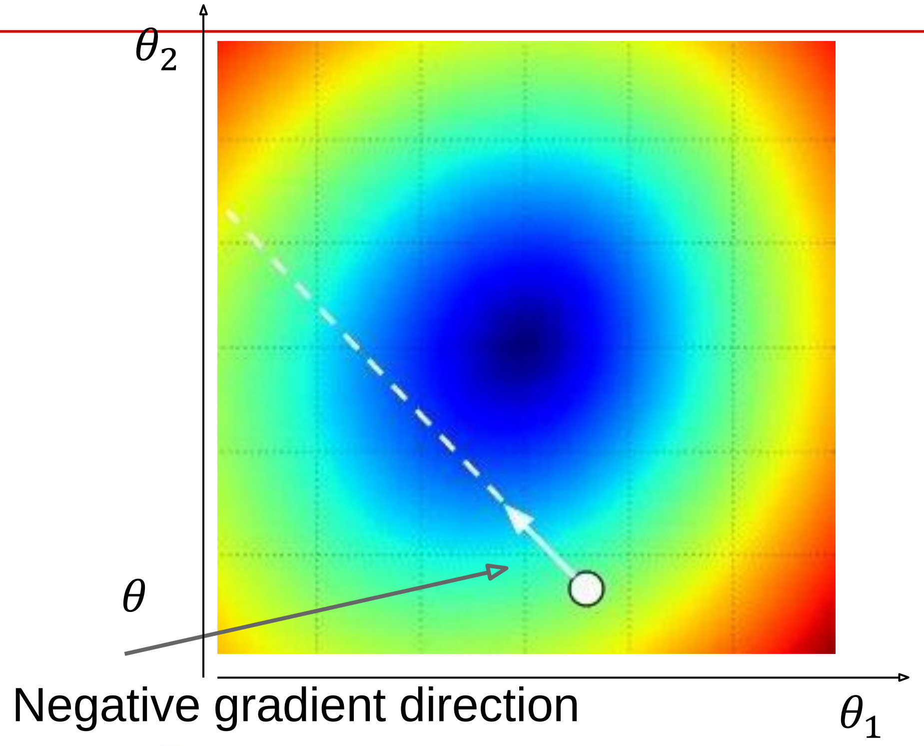


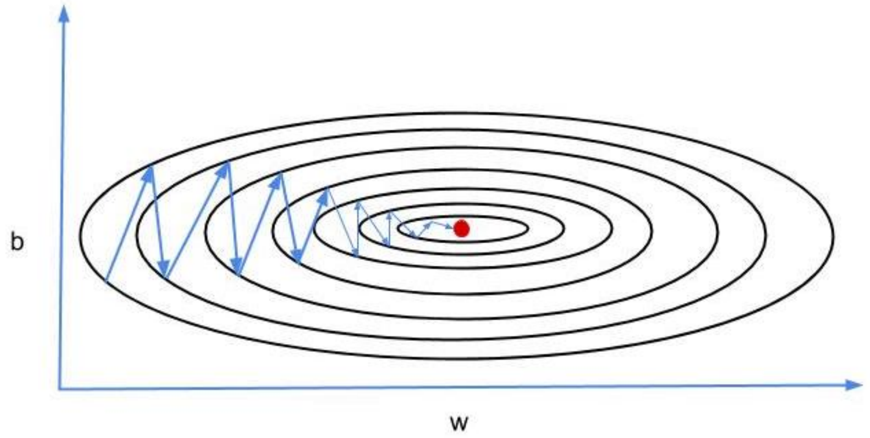
$$\mathbb{E}_{(x,y)\sim D}\mathrm{Loss}(x, y; \theta)$$



Gradient Descent

- Steepest descent may result in inefficient 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

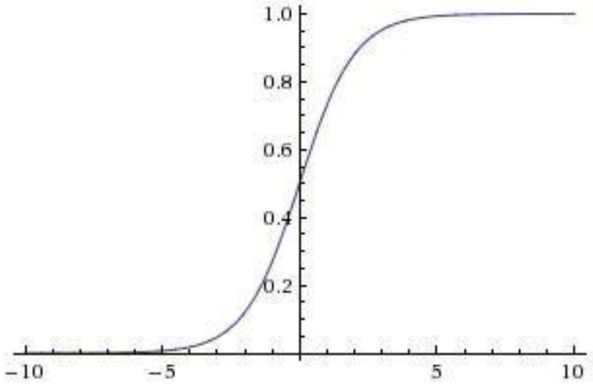




http://dataplusplus.ca/blog/2017/gradient-descent-with-momentum

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 γ, β 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: $\mathcal{B} = \{x_{1\dots m}\}$;
Parameters to be learned: γ, β

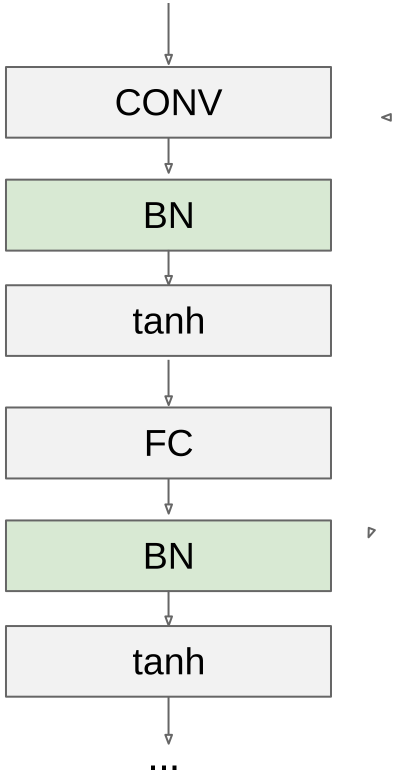
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

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

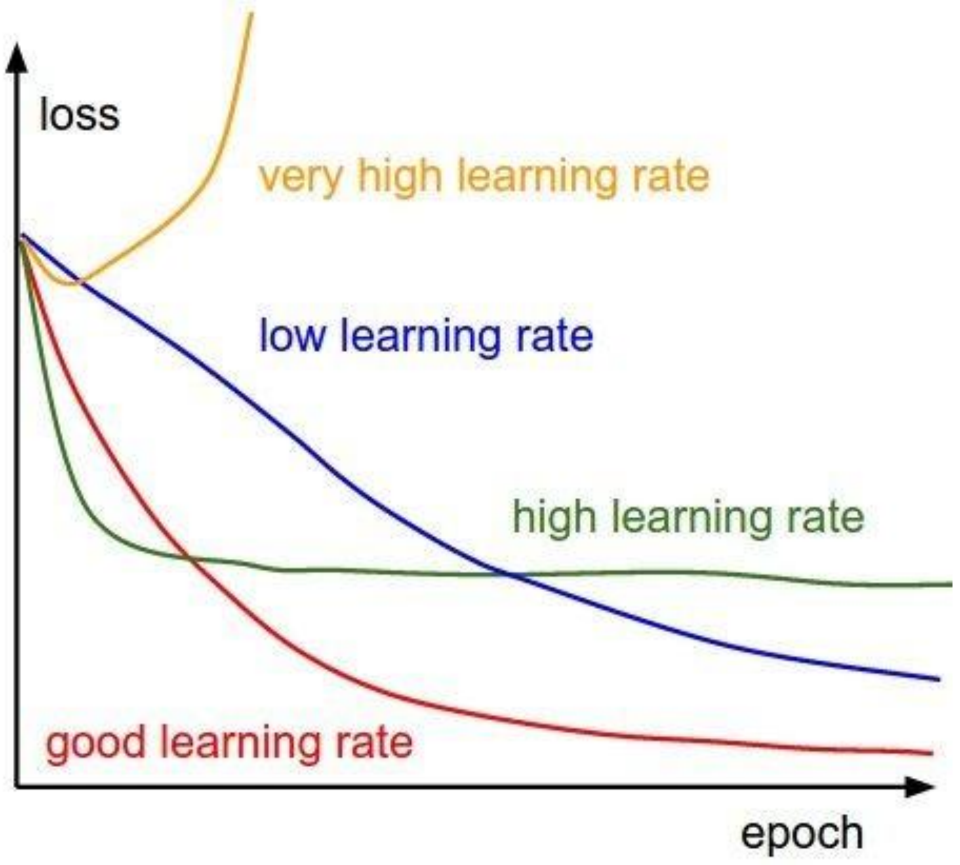
$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

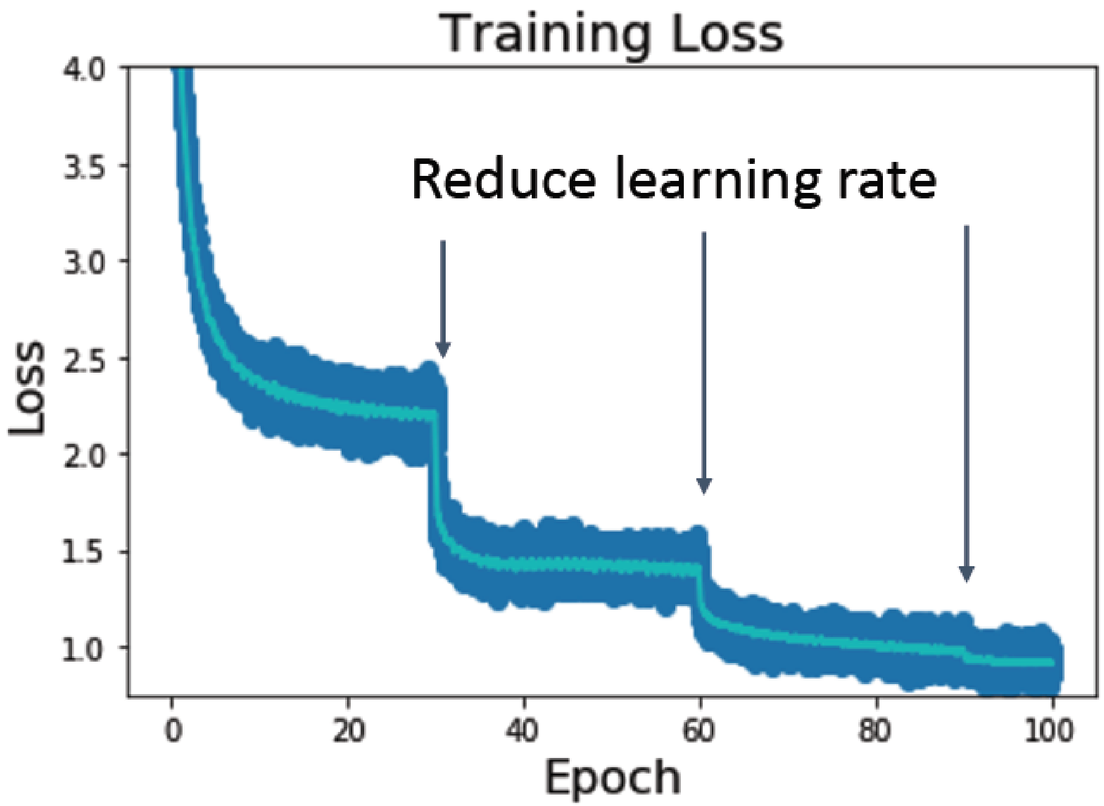
$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

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



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
  - If a function f of two variables can be approximated by another function of one variable ($f(x_1, x_2) \approx g(x_1)$), then we say that f has a low effective dimension. Fig. 1 illustrates how point grids and uniformly random point sets differ in how they cope with low effective dimensionality

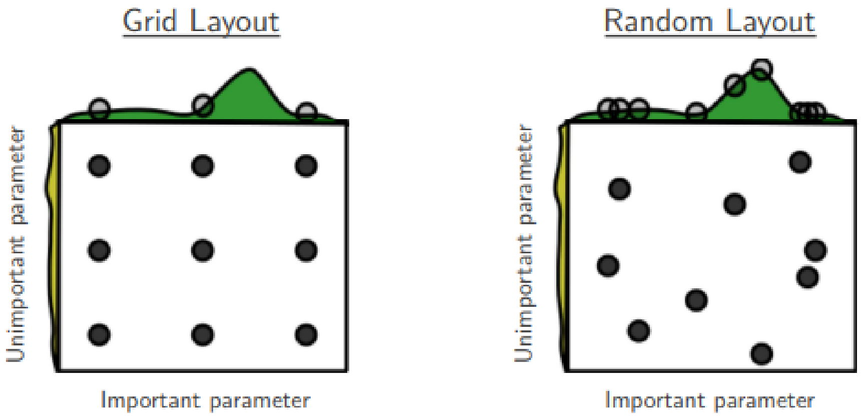
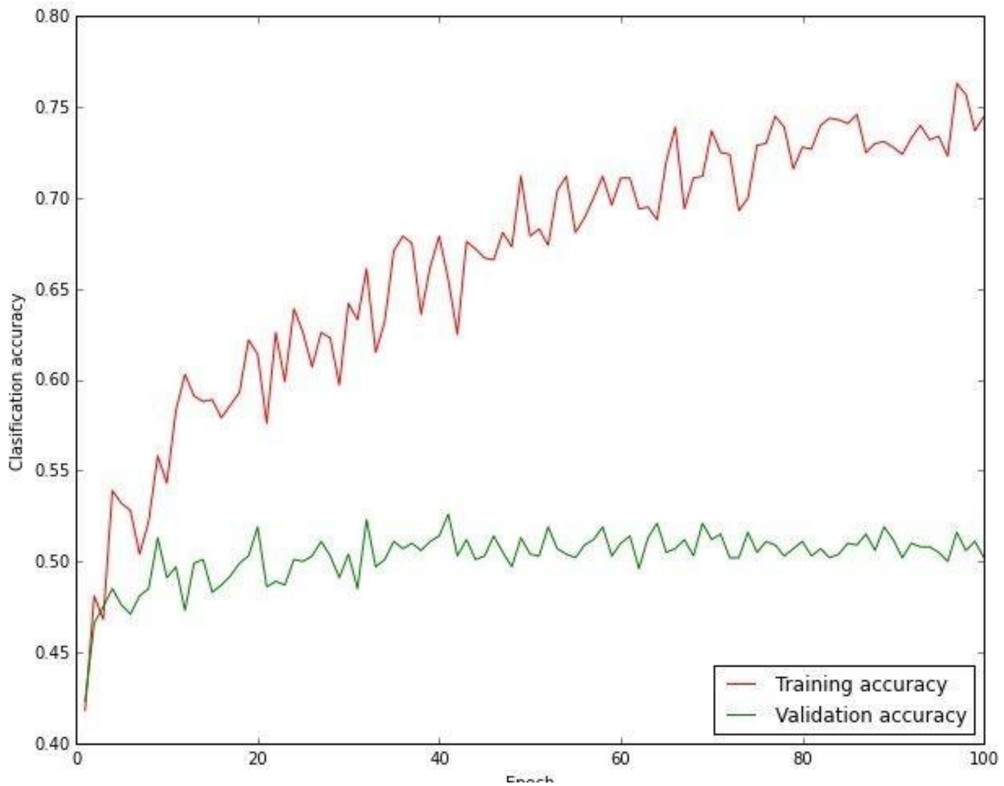


Figure 1: Grid and random search of nine trials for optimizing a function $f(x,y) = g(x) + h(y) \approx g(x)$ with low effective dimensionality. Above each square $g(x)$ is shown in green, and left of each square $h(y)$ is shown in yellow. With grid search, nine trials only test $g(x)$ in three distinct places. With random search, all nine trials explore distinct values of g. This failure of grid search is the rule rather than the exception in high dimensional hyper-parameter optimization.

Bergstra, James, and Yoshua Bengio. "Random search for hyper-parameter optimization." *Journal of machine learning research* 13.2 (2012).

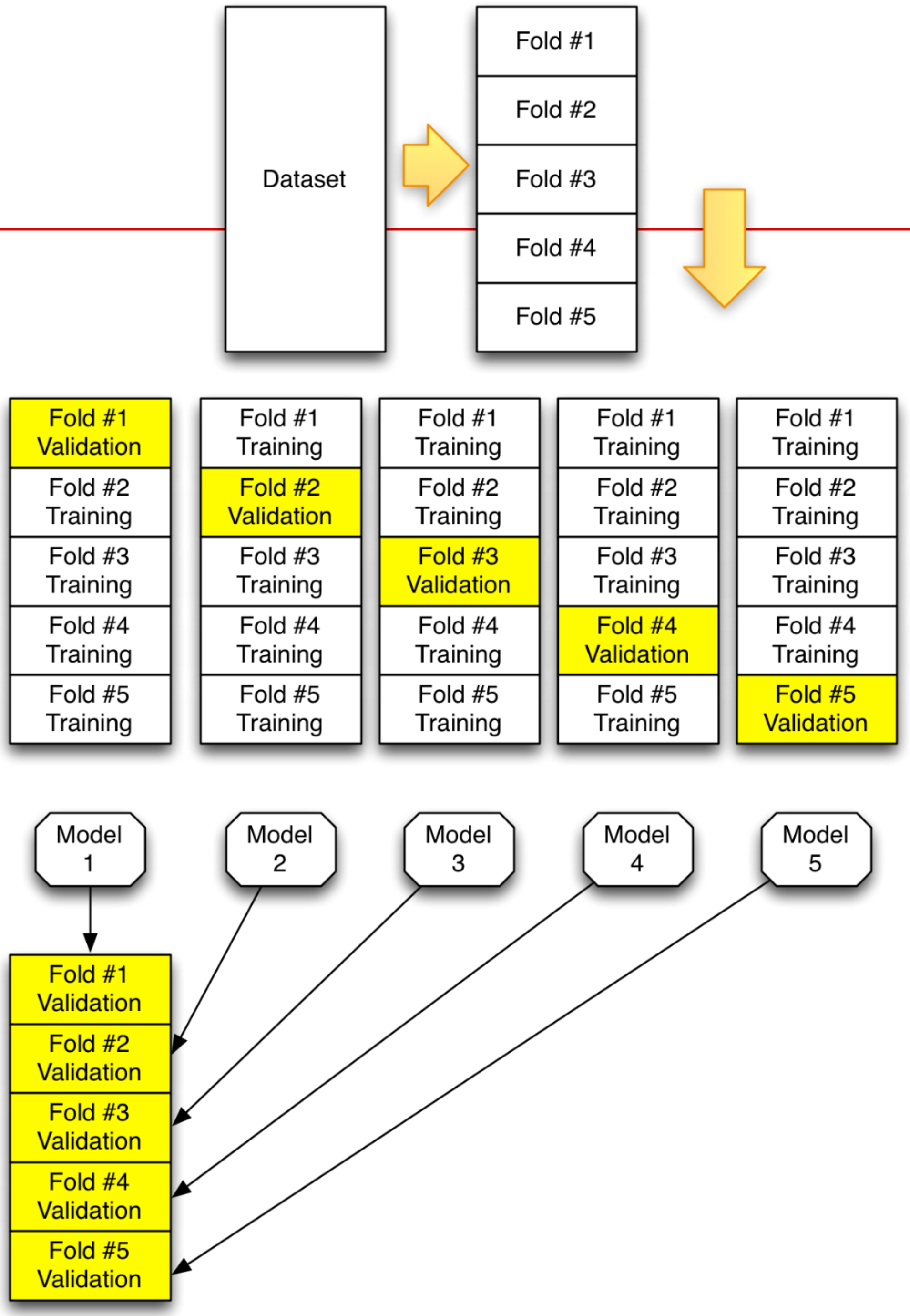
Classification Accuracy

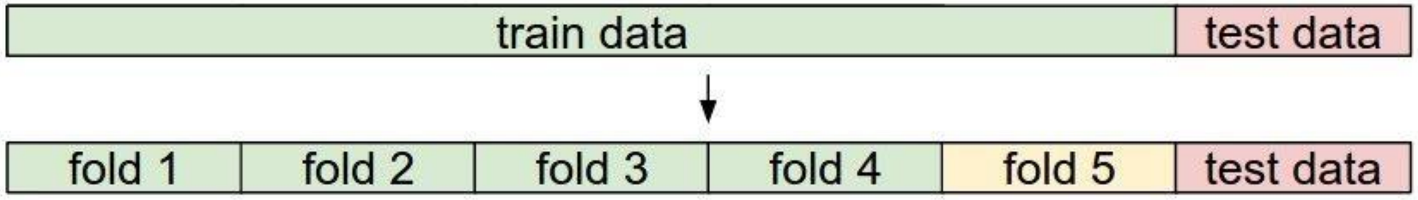
- Big gap between training accuracy and validation accuracy may imply overfitting => decrease model capacity/size
- No gap may imply underfitting => increase model capacity/size



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





https://github.com/jeffheaton/t81_558_deep_learning/blob/master/t81_558_class_05_2_kfold.ipynb

Data Augmentation for Enlarging Training Dataset

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