MSBA 434: Advanced Workshop on Machine Learning

Lecture 5: Ensemble Methods

UCLA Anderson

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2019

Agenda

1. Why ensembles work?
2. Ensemble techniques
3. Case Study: Gaussian Circles

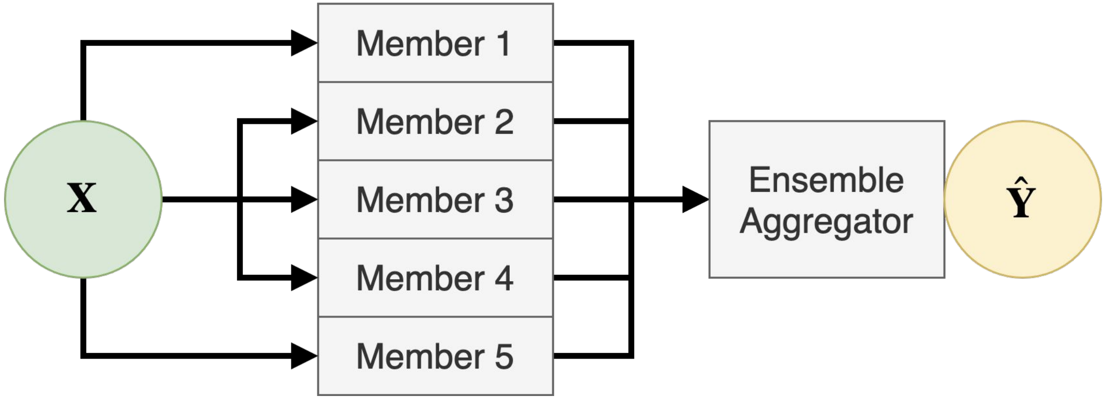
4. Final Project
5. Course Summary
6. Feedback Session

Ensemble Inference

Ensemble is a collection of models whose output is aggregated together.

Under certain conditions, aggregated output is better than any member output.

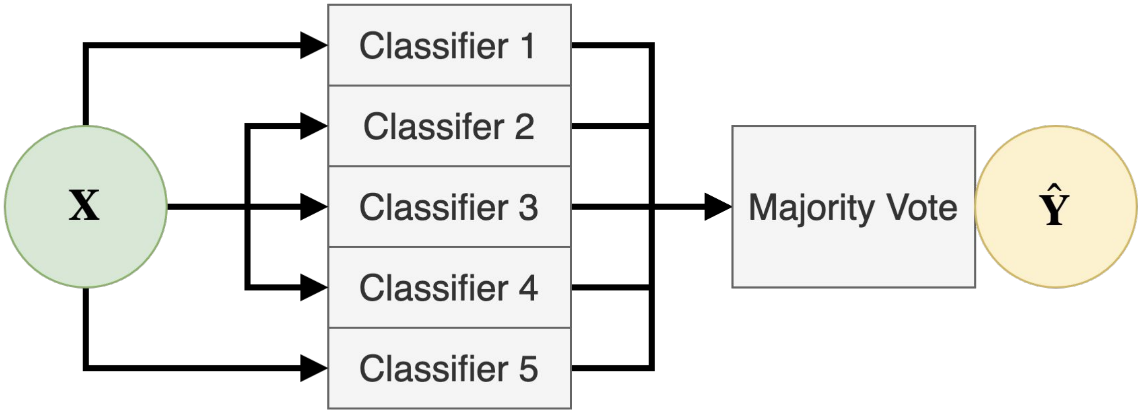
Members may or may not communicate.



Binary Classification

Ensemble output is the class predicted by the majority of member classifiers.

In case of probabilities, the average probability will be consistent with discrete majority vote.

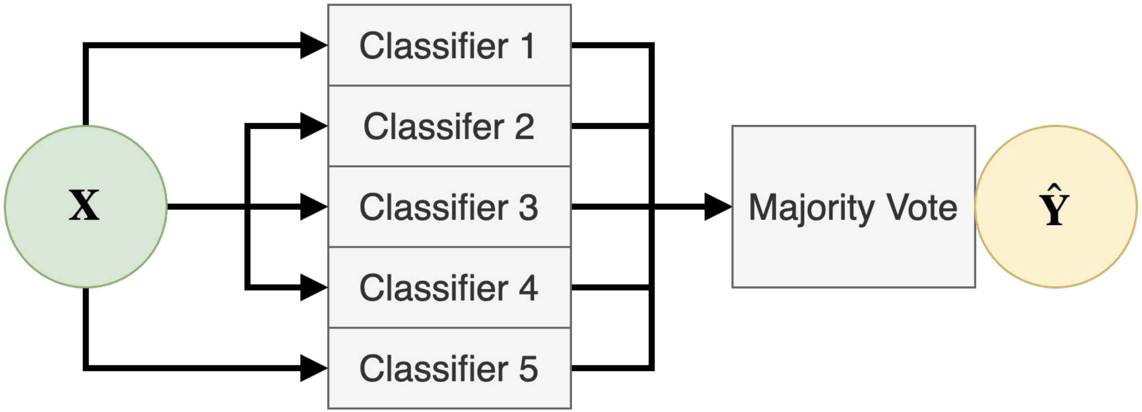


Ensemble Properties

Ensemble performance depends on:

1. Member strength
2. Ensemble size
3. Member independence

Ensemble performance may or may not be better than its best member.



Ensemble Performance

How to evaluate ensemble performance as a function of its properties?

Method 1: Analytical
Mathematical analysis of the statistical distribution and its properties.

Method 2: Monte Carlo
Approximate the distribution properties using a finite batch of random samples.

See MonteCarlo.ipynb for NumPy implementation.

$$x \sim p_{data}$$

$$a_i(x) \in \mathbb{R}^n \rightarrow \{0, 1\}$$

$$a_i(x) \sim \text{Bernoulli}(p)$$

$$\mathbb{E}[\ a_i(x)\ ] = p$$

$$e(x) = \lceil \sum_i^s \frac{a_i(x)}{s} \rfloor$$

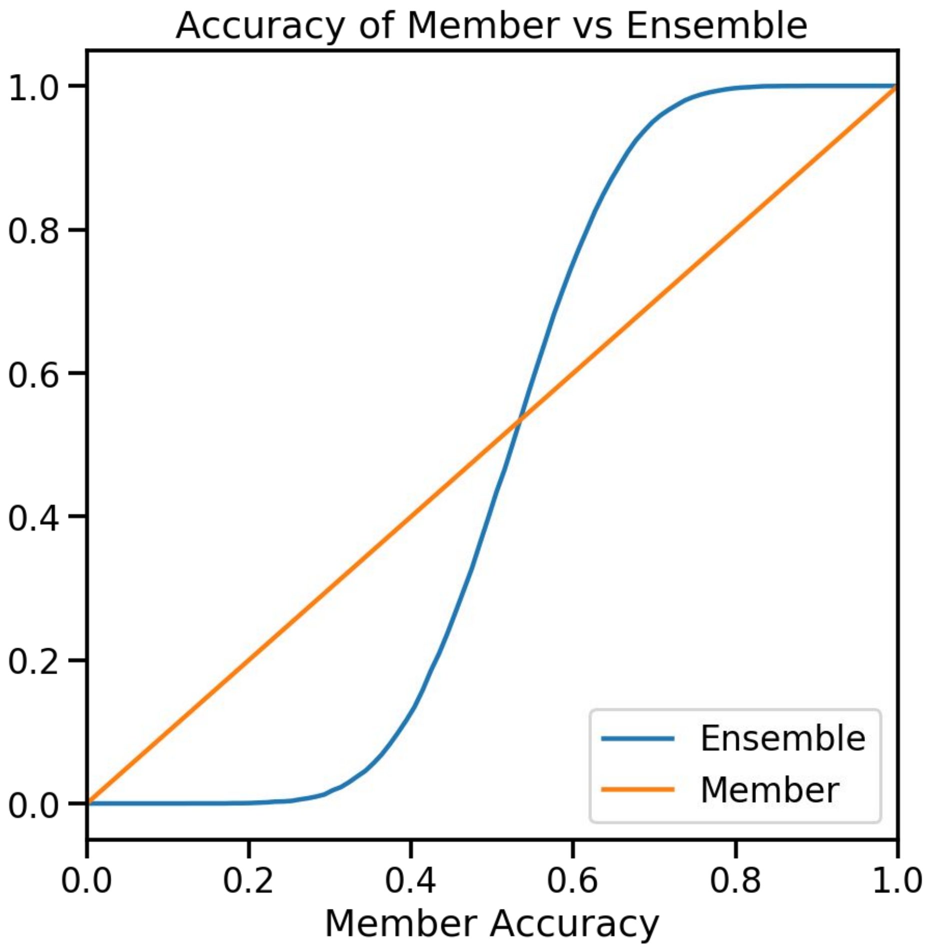
$$e(x) \sim \text{Binomial}(p, s) > \frac{s}{2}$$

Member Strength

Simulation
Ensemble of 20 independent binary classifiers.

Inference
Ensemble strength increases with member strength.

Ensemble members must be better than random.

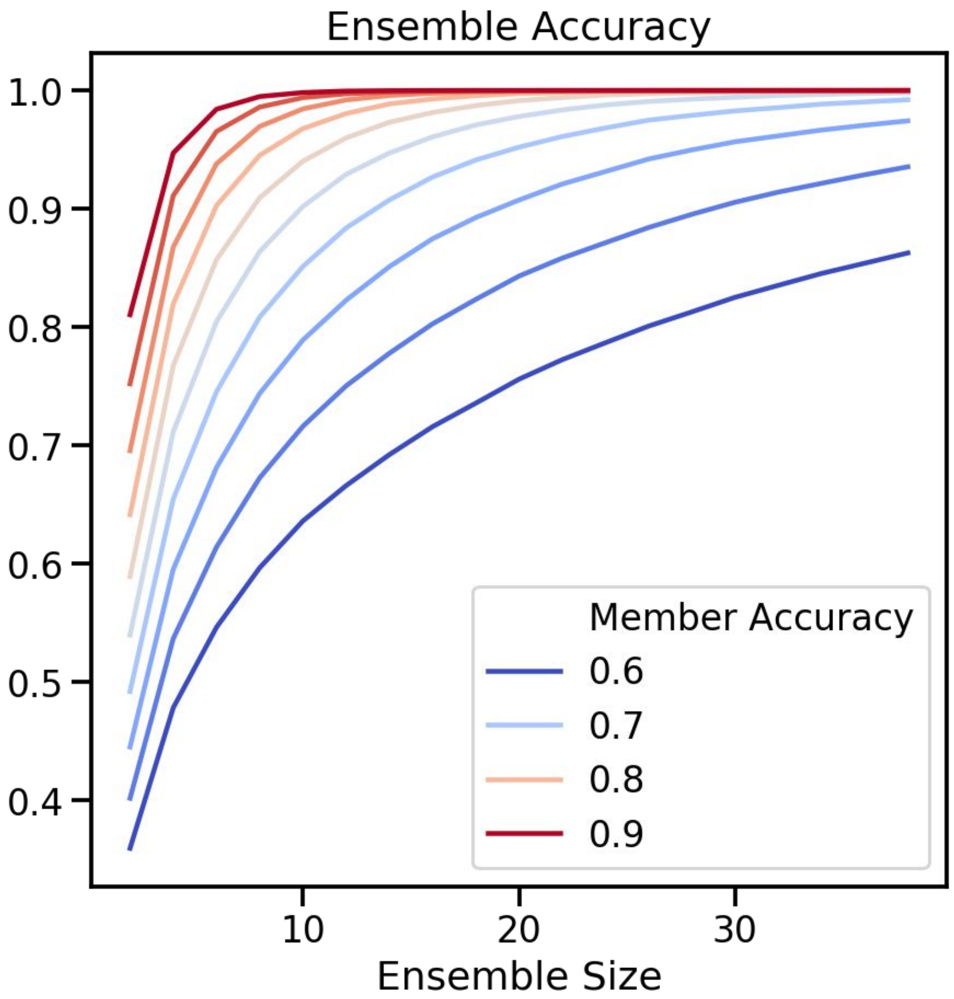


Ensemble Size

Simulation
Ensemble of independent binary classifiers.

Inference
Ensemble strength increases with size.

Marginal value of an additional member decreases with its accuracy and ensemble size.



Member Independence

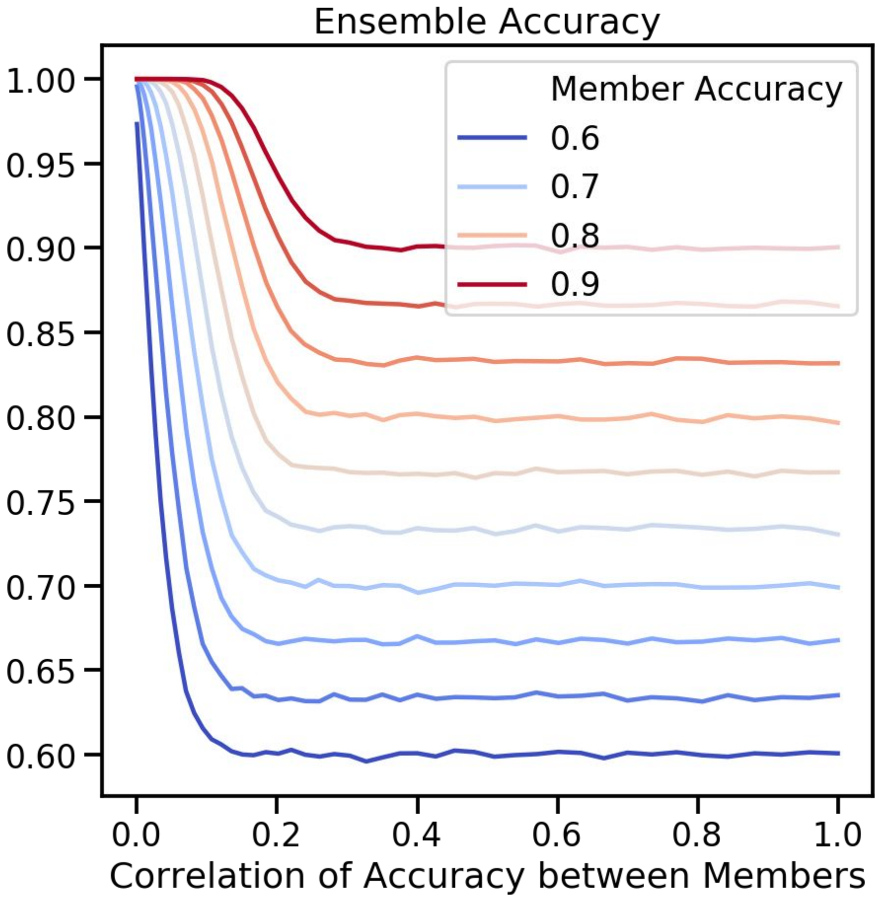
Simulation

Ensemble of 100 binary classifiers with correlated errors.

Inference

Ensemble strength decreases with correlation between members.

Sensitivity to correlation decrease with member strength.

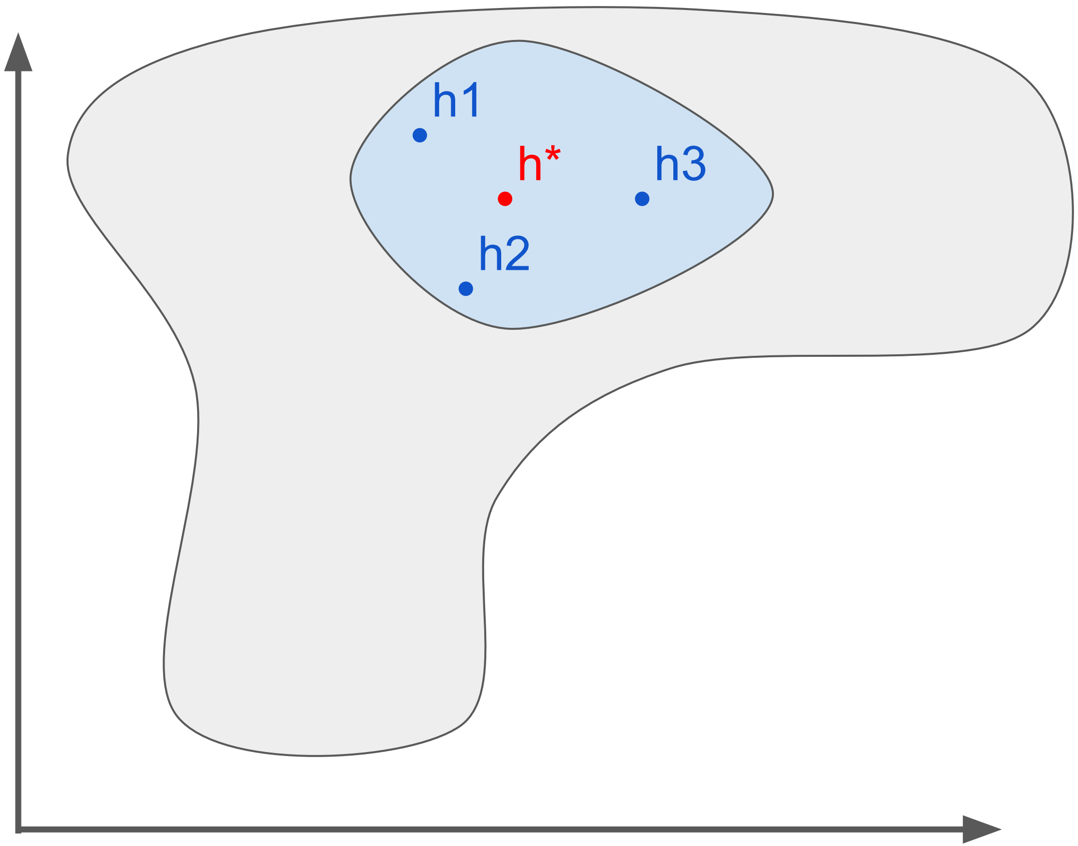


See MonteCarlo.ipynb for NumPy implementation.

Statistical

When datasets are small relative to the hypothesis space, multiple hypotheses may minimize the estimate of the cost.

However, under all possible datasets, there should be a single optimal hypothesis.

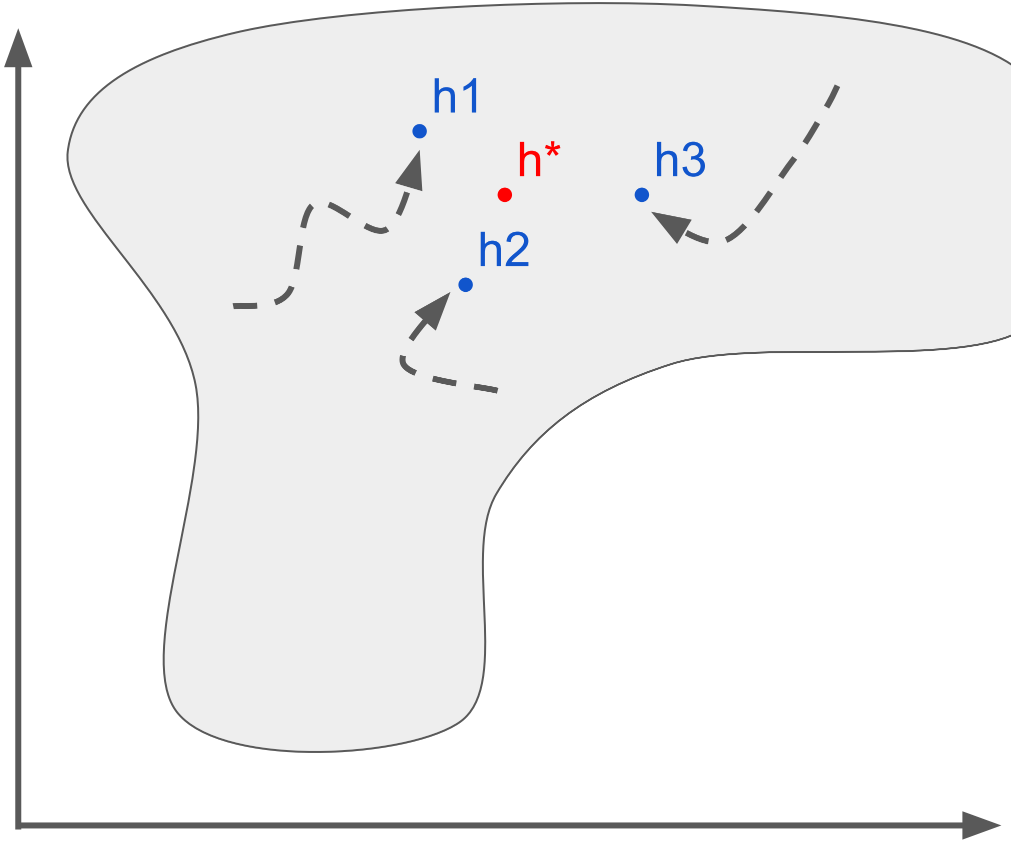


Diettrich, T. G. (2000)

Computational

Iterative learning algorithms (e.g. gradient descent) may converge to different local minima.

An average of multiple hypotheses may be close to the global minimum.

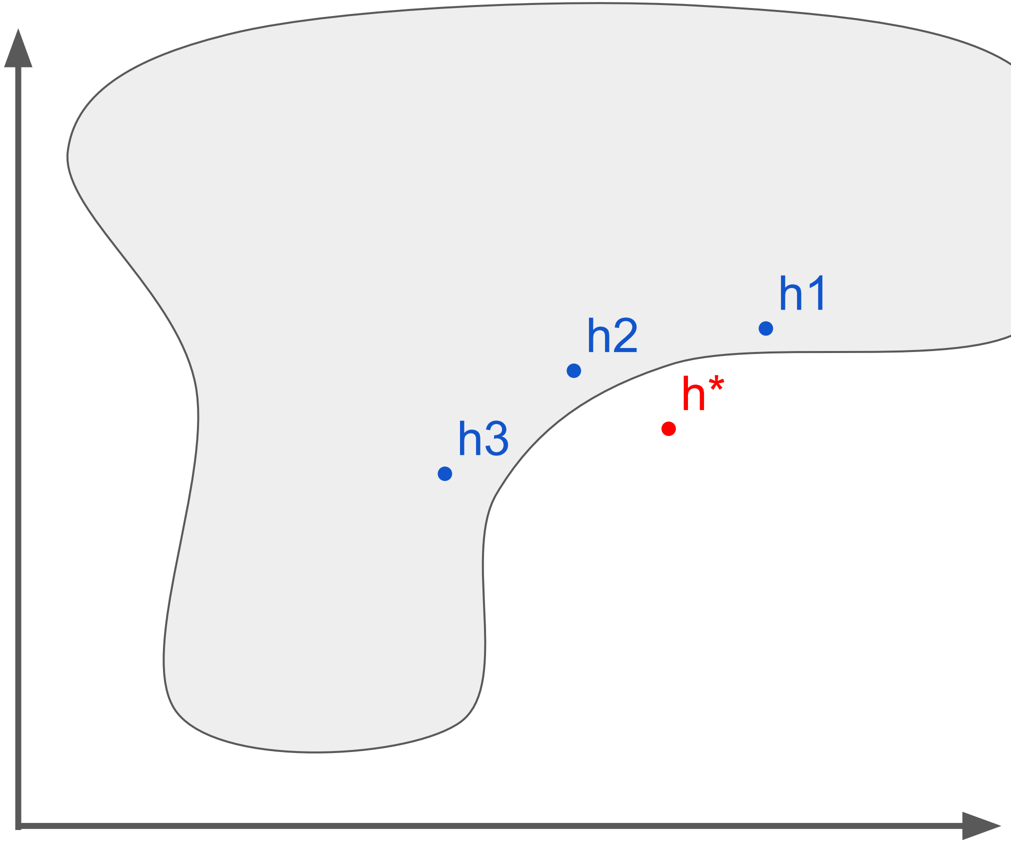


Diettrich, T. G. (2000)

Representational

The optimal hypothesis may be outside of the effective hypothesis space that is searched over using a finite dataset.

An average of multiple hypotheses may be outside of the effective hypothesis space and closer to the optimal hypothesis.



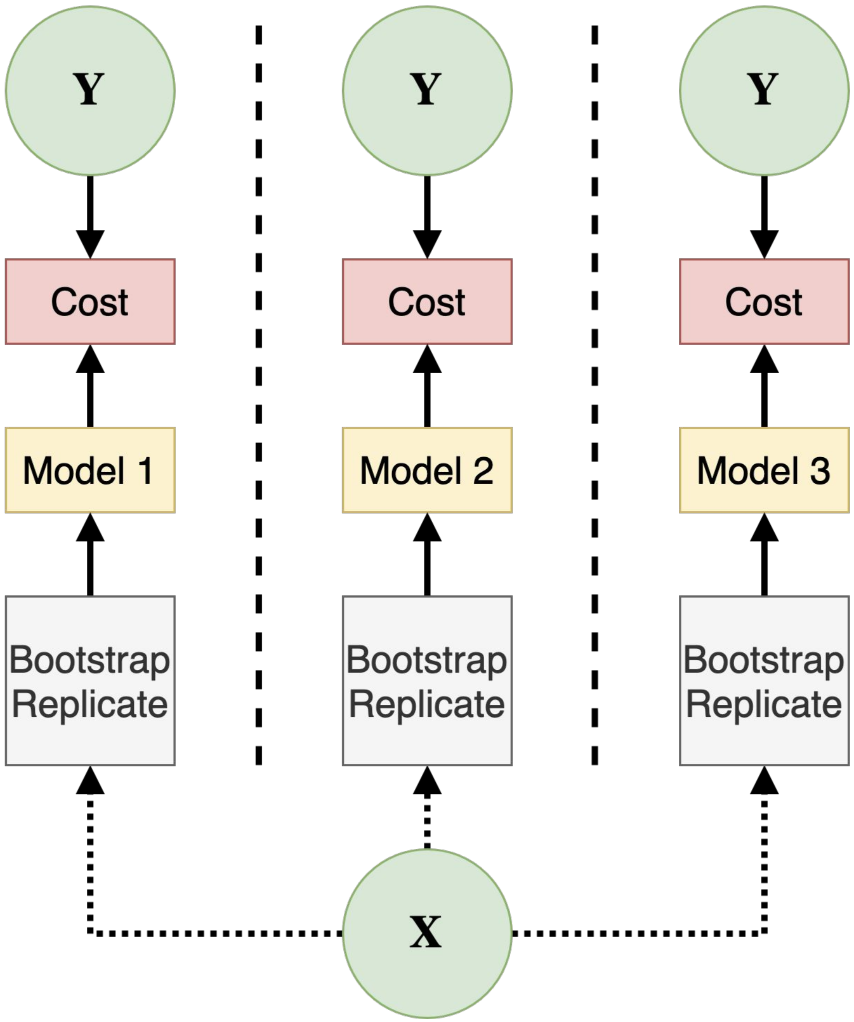
Diettrich, T. G. (2000)

Bagging

Bootstrap replicate = random resampling of the dataset with replacement.

Bootstrap aggregation = an ensemble of models trained on different bootstrap replicates.

On average ~60% of data present in every replicate.

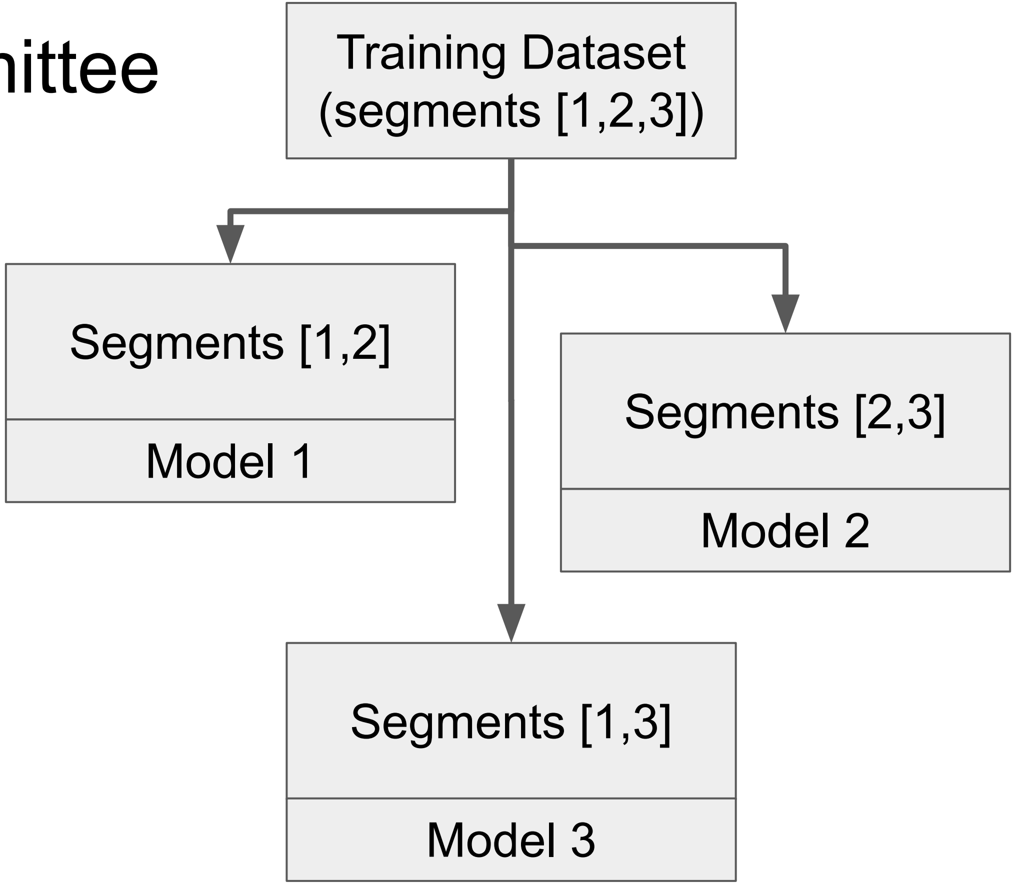


Diettrich, T. G. (2000)

Cross-validated Committee

Segments = n disjoint subsets of the dataset.

Cross-validated committee = an ensemble of n-1 models trained on the dataset with different segments missing.

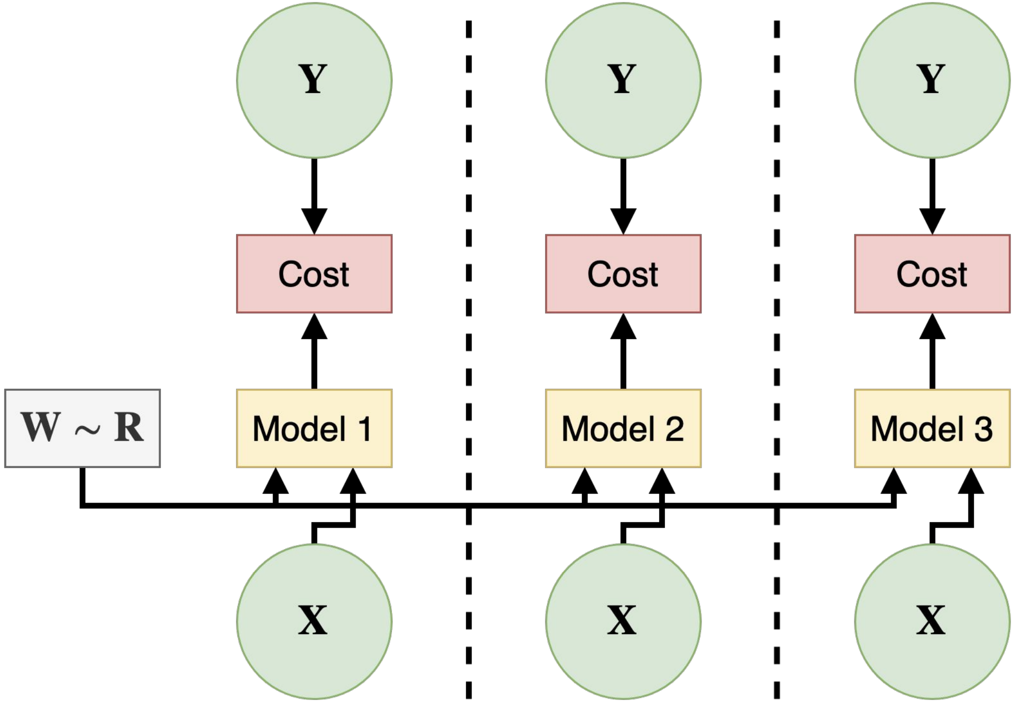


Diettrich, T. G. (2000)

Noise Injection: Initialization

Create multiple neural networks with different initial parameters.

After training, the networks will arrive at different hypotheses.



Diettrich, T. G. (2000)

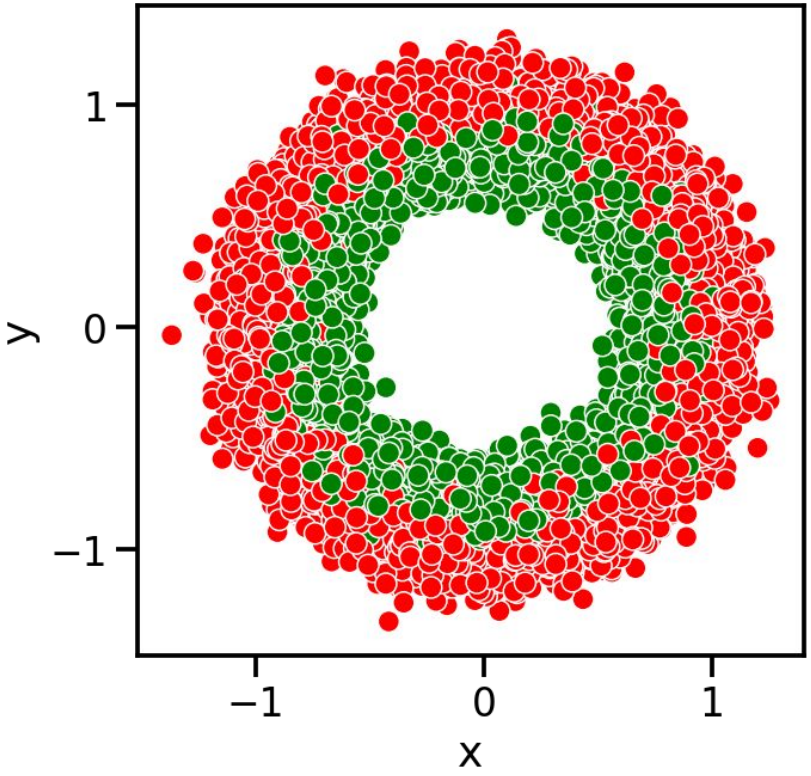
Case Study: Gaussian Circles

Dataset

Collection of 10K points in 2D space arranged as two circles with Gaussian noise.

Task

Classify a point as either green or red given its coordinates.



Logistic Regression #1

Features

Coordinates X, Y, and constant

Target

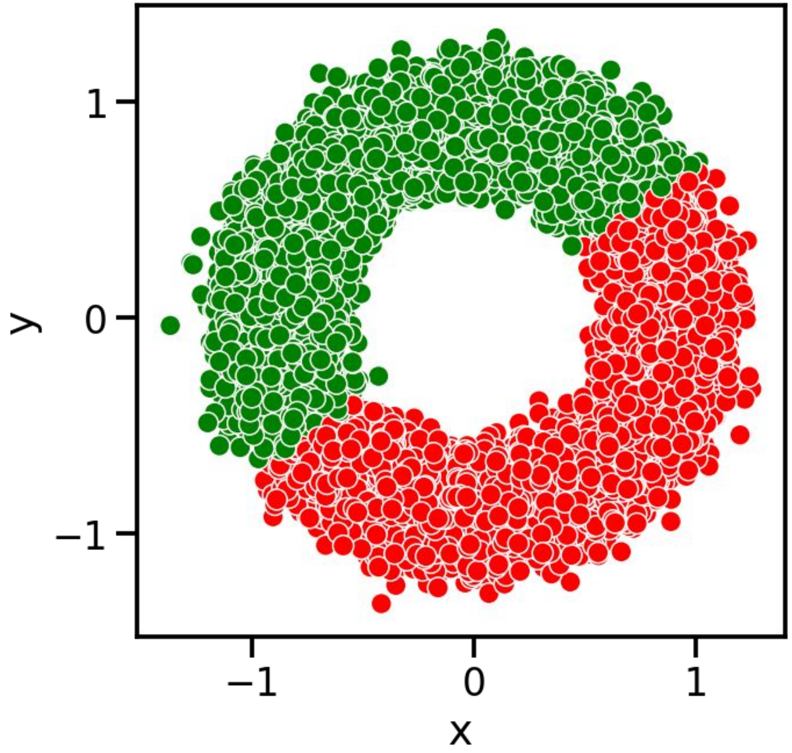
Red = 0, green = 1

Accuracy

0.50

Log Loss

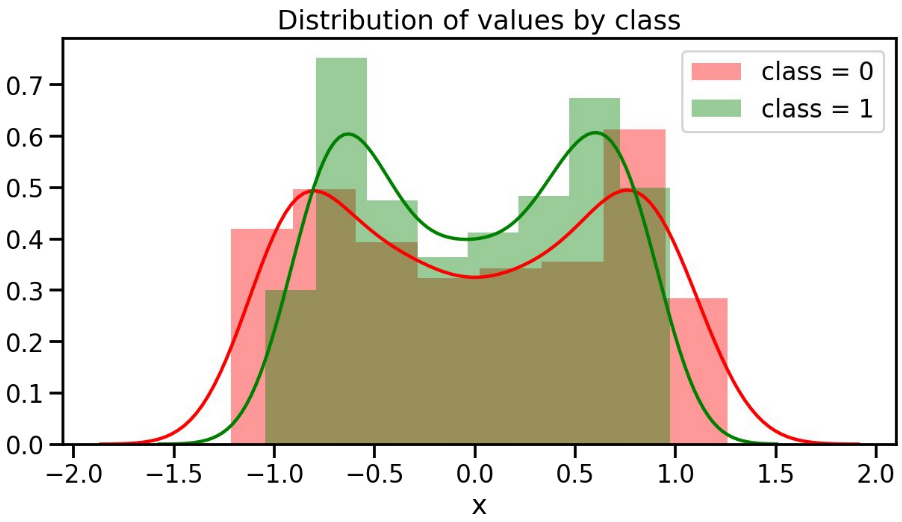
0.693

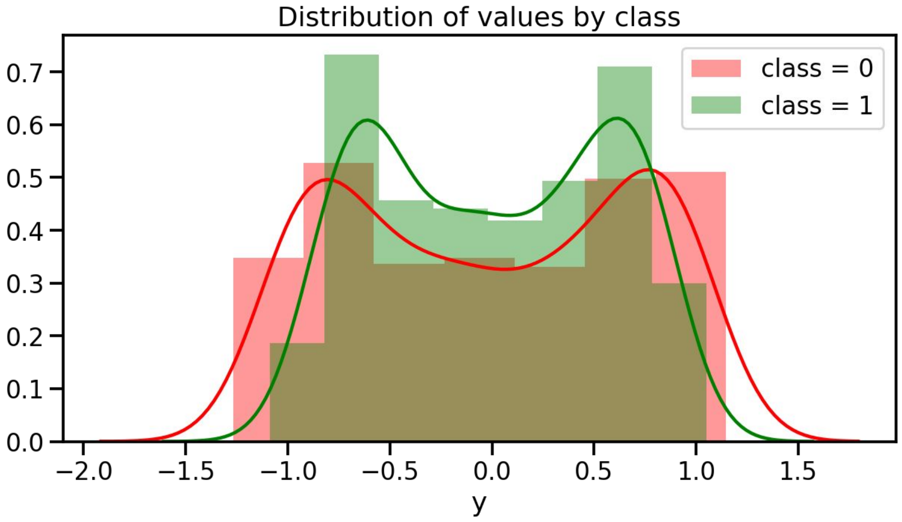


Distribution by X and Y

Inference from Distributions
There is no way to separate classes with a straight line in either X or Y space.

How to construct **a feature which can separate the two circles** with a line?



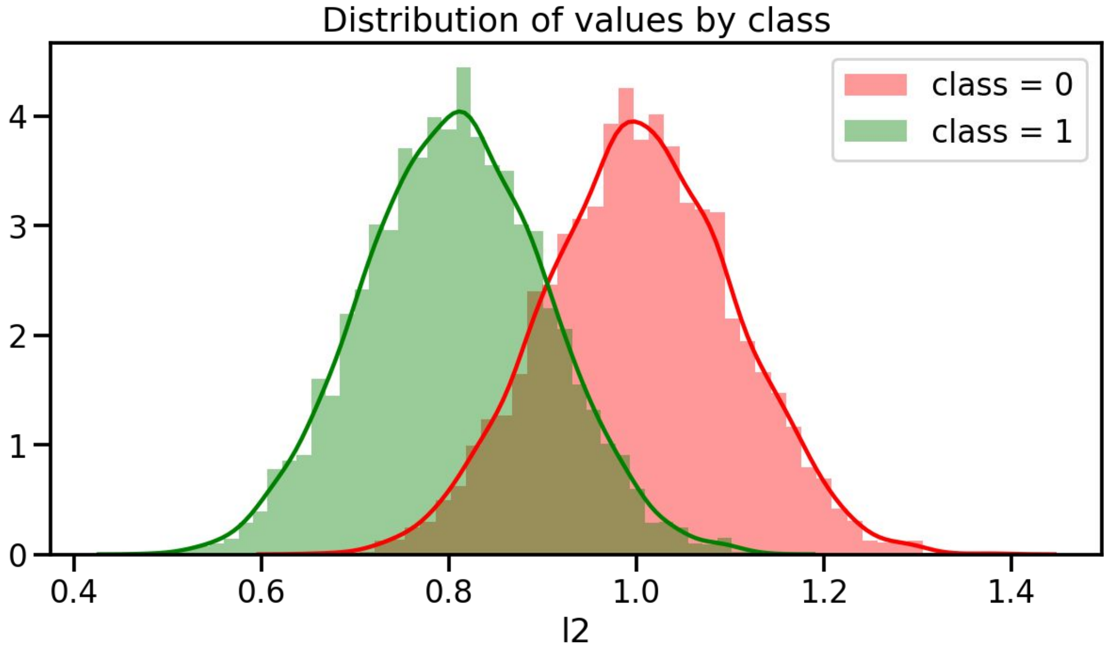


Distribution by L2 Norm

L2 Norm of X and Y = distance from the center.

Distributions **partially separated** from each other.

Overlapping area implies that a **perfectly accurate classifier is not possible**.



Logistic Regression #2

Features

L2 norm, and constant

Target

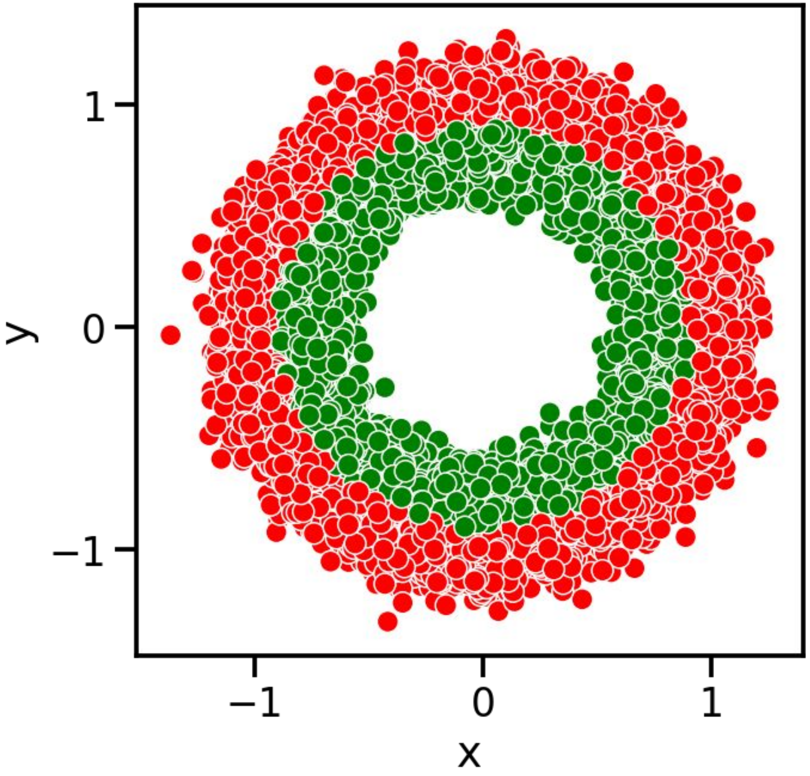
Red = 0, green = 1

Accuracy

0.84

Log Loss

0.36



Neural Network

Layers

1. FC with 10 nodes, tanh
2. FC with 1 node, sigmoid

Features

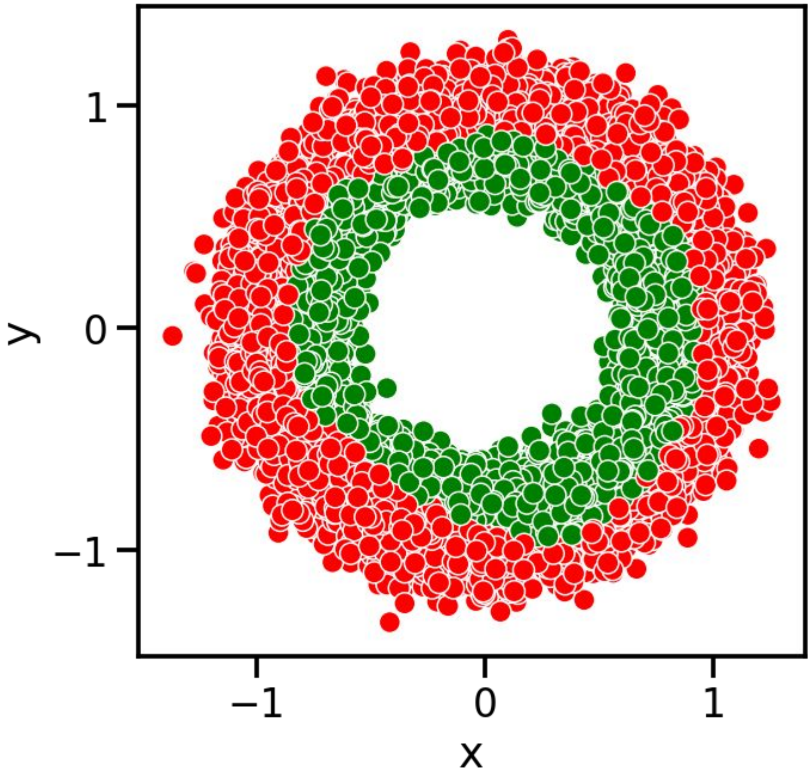
Coordinates of X and Y

Target

Red = 0, green = 1

Log Loss

0.435

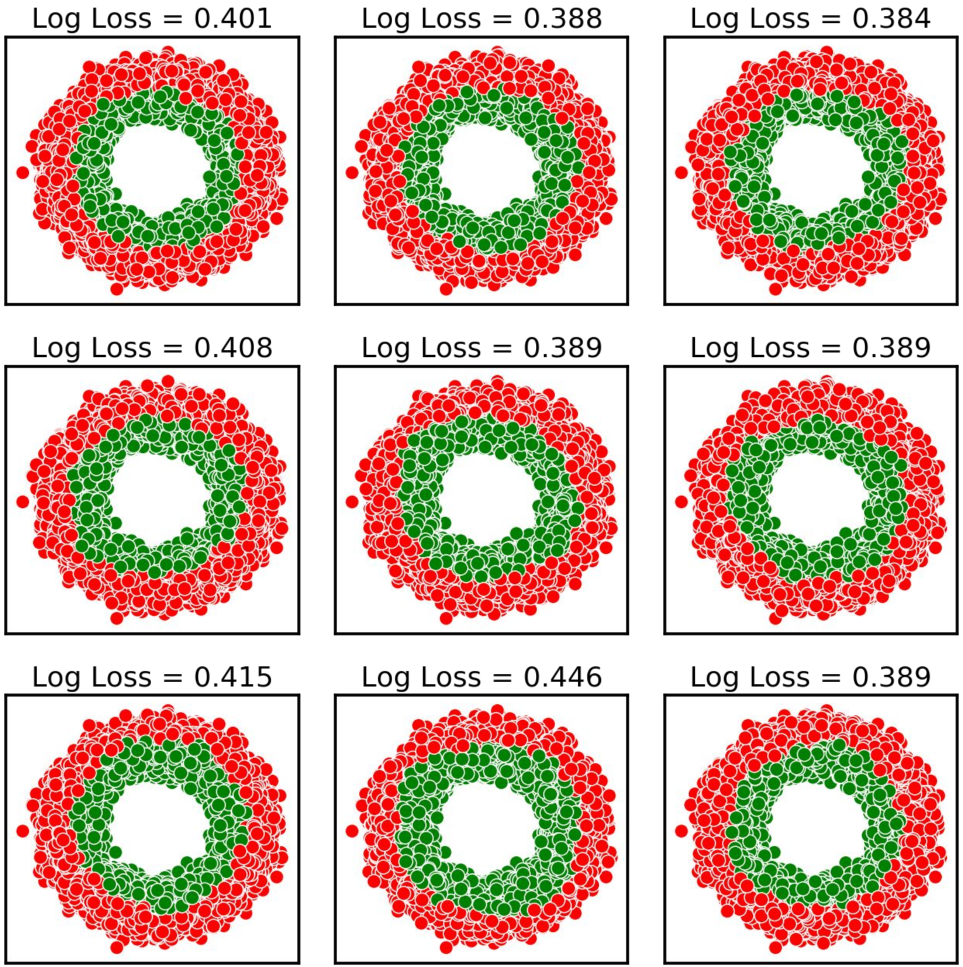


Example: Initialization

1. Sample 9 different initialization seeds

2. Train each model for 10 epochs

3. Compare performance on the training dataset



Ensemble: Initialization

Members of Ensemble

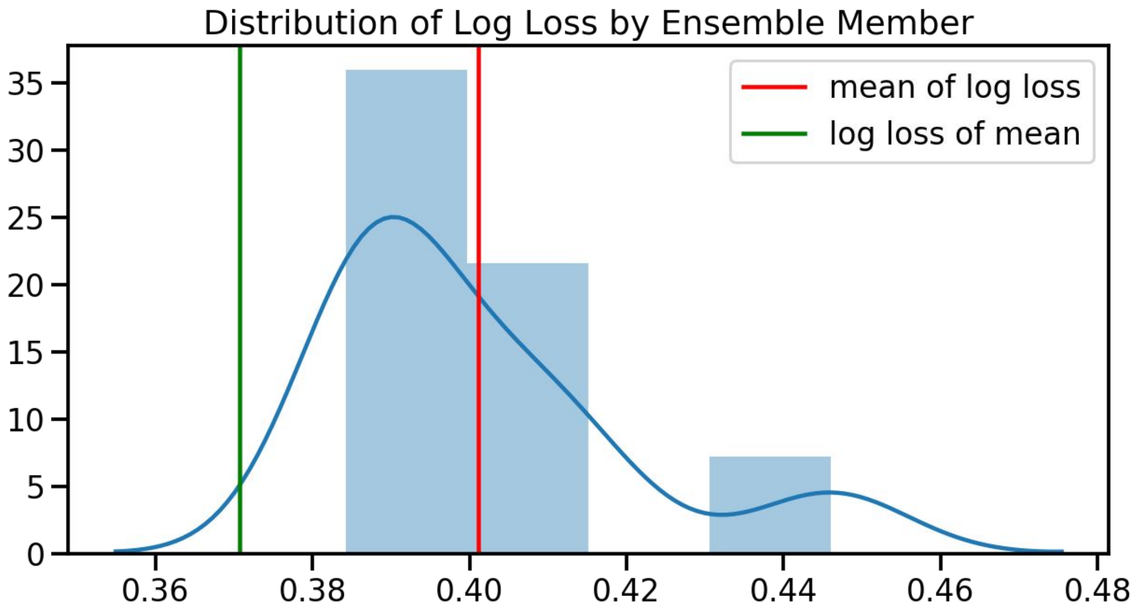
9 neural networks with different weight initializations

Aggregation Method

Average of Probability

Log Loss of Ensemble

0.371

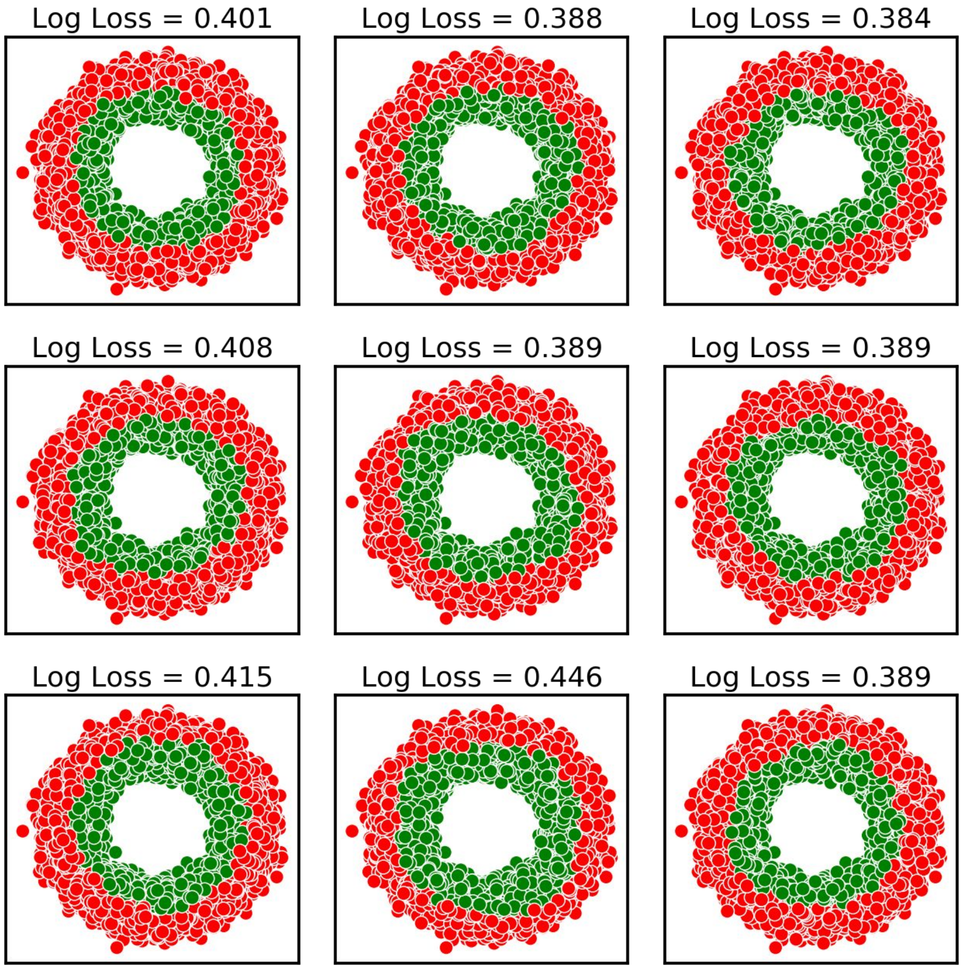


Example: Bagging

1. Sample 20 different bootstrap replicates of the training dataset

2. Train each model for 10 epochs

3. Compare performance on the training dataset



Ensemble: Bagging

Members of Ensemble

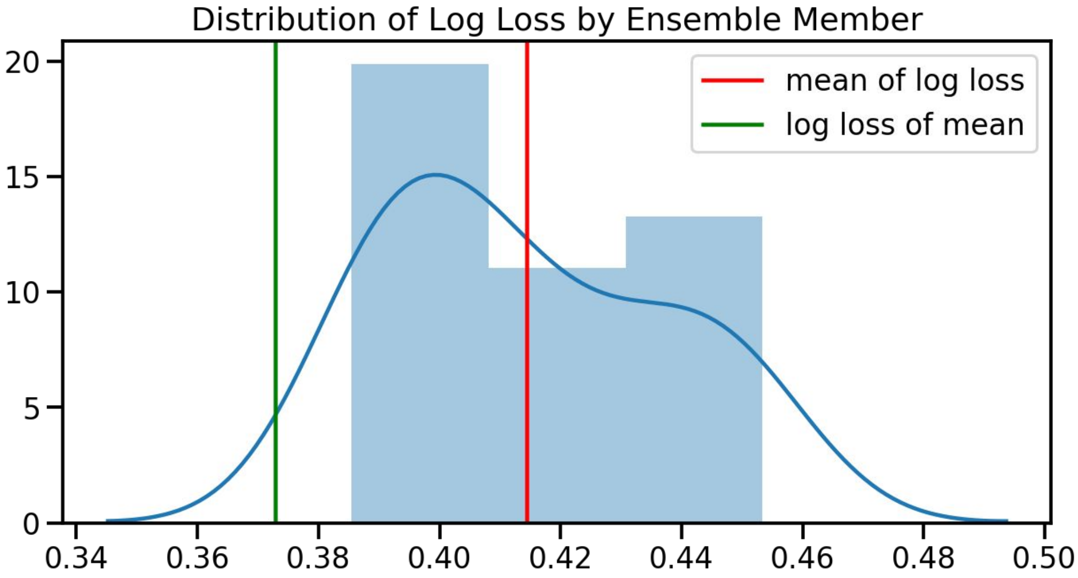
20 neural networks with different training bags

Aggregation Method

Average of Probability

Log Loss of Ensemble

0.373

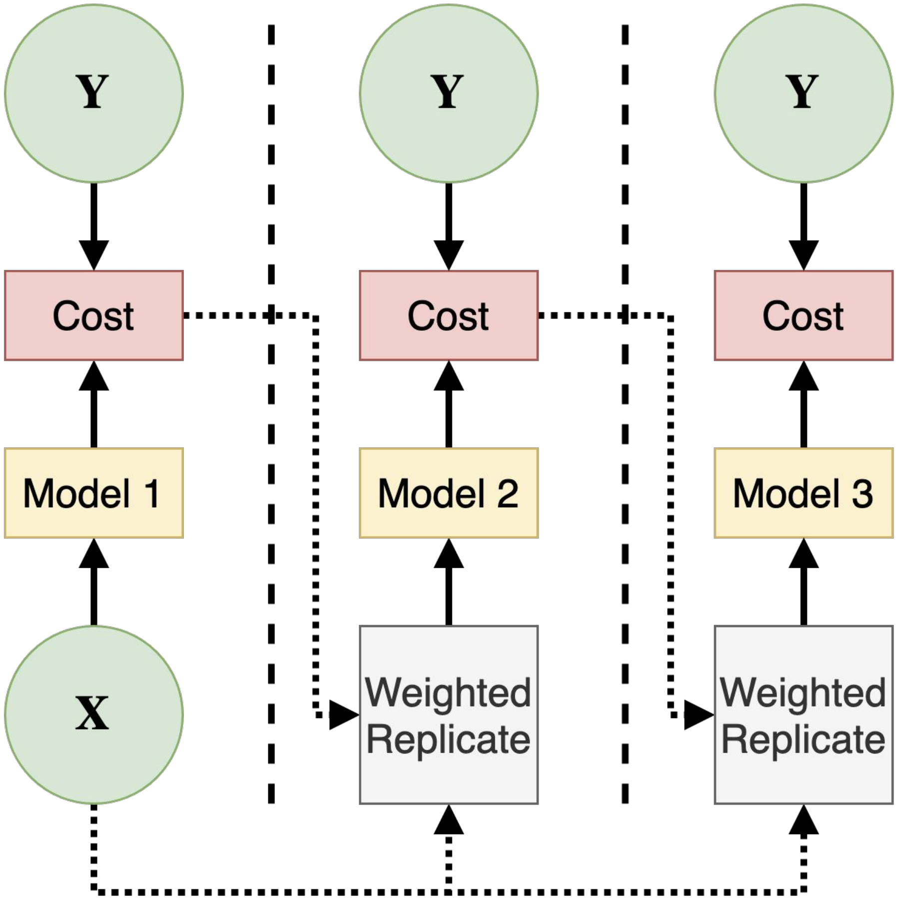


AdaBoost: Training #1

Sequential model training on different datasets.

Each dataset resampled with probabilities depending on the per-sample cost of the previous model.

Each subsequent model is trained with higher focus on hard training samples.



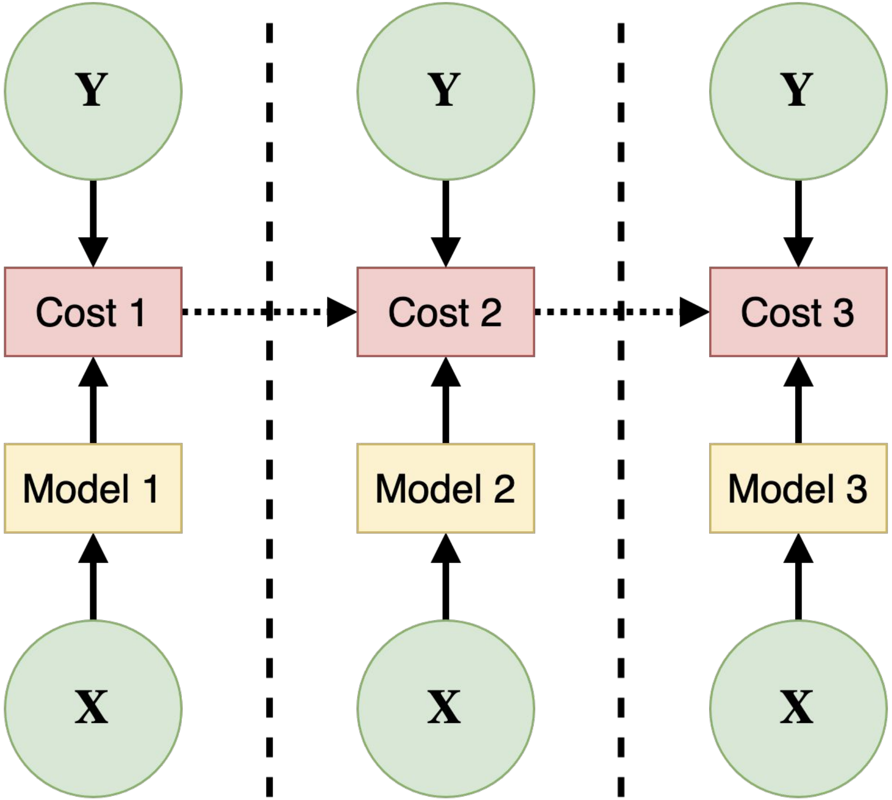
Shwenk, H., Bengio, Y. (2000)

AdaBoost: Training #2

Sequential model training on the same dataset.

Cost = average of this model's per-example cost weighted by per-example cost from the previous model.

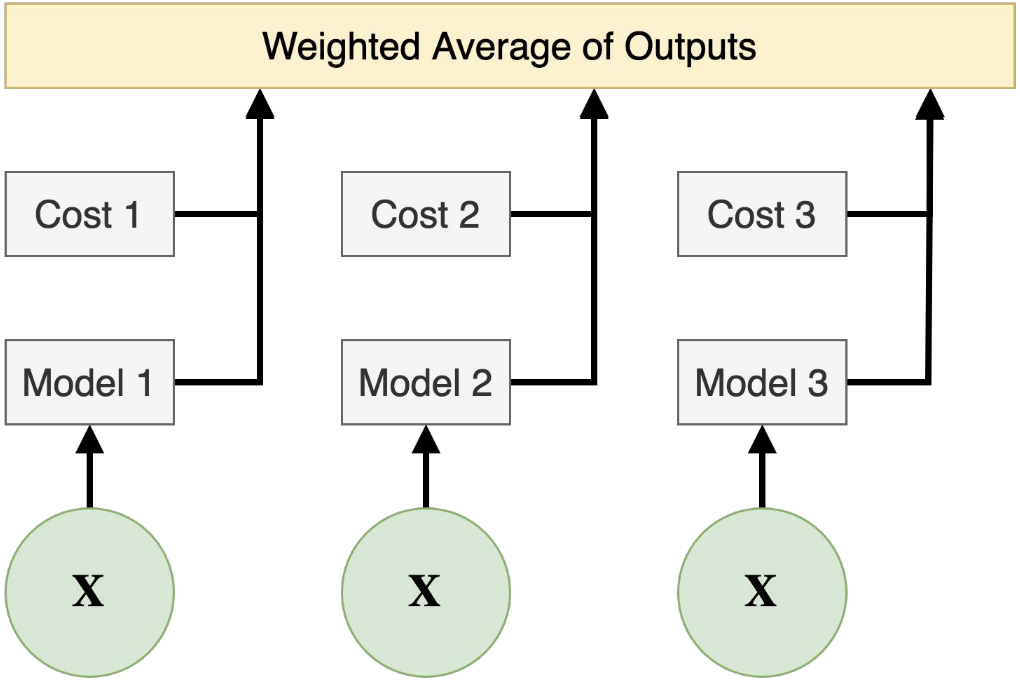
Each subsequent model is trained with higher focus on hard training examples.



Shwenk, H., Bengio, Y. (2000)

AdaBoost: Inference

Ensemble output is the average over each model's output weighted by the performance on the training dataset.

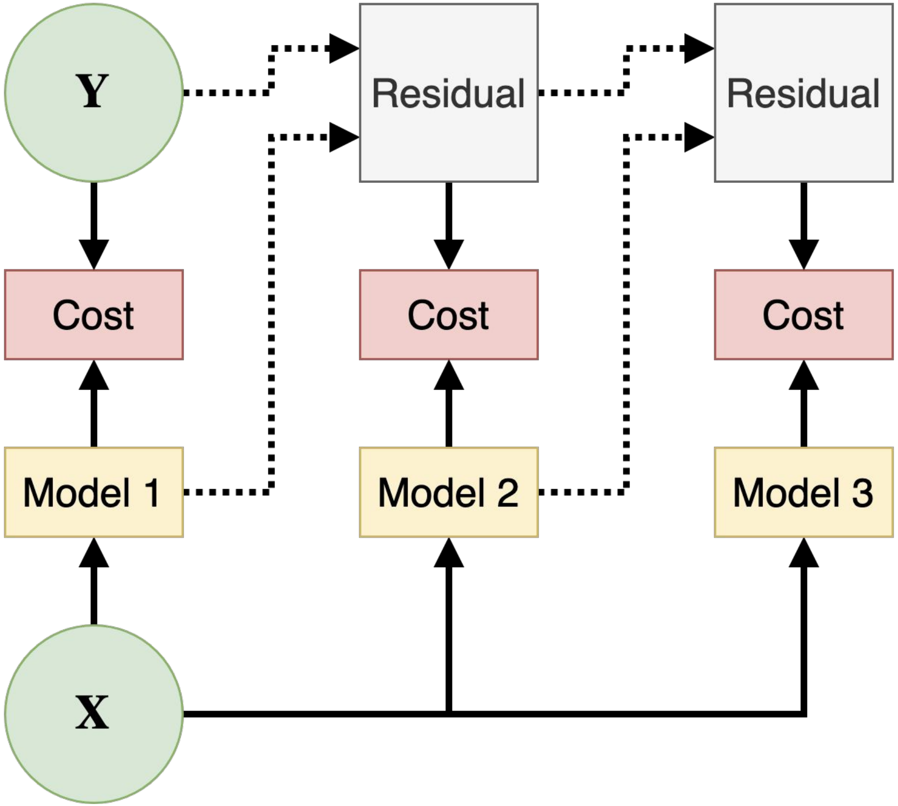


Shwenk, H., Bengio, Y. (2000)

Gradient Boosting: Training

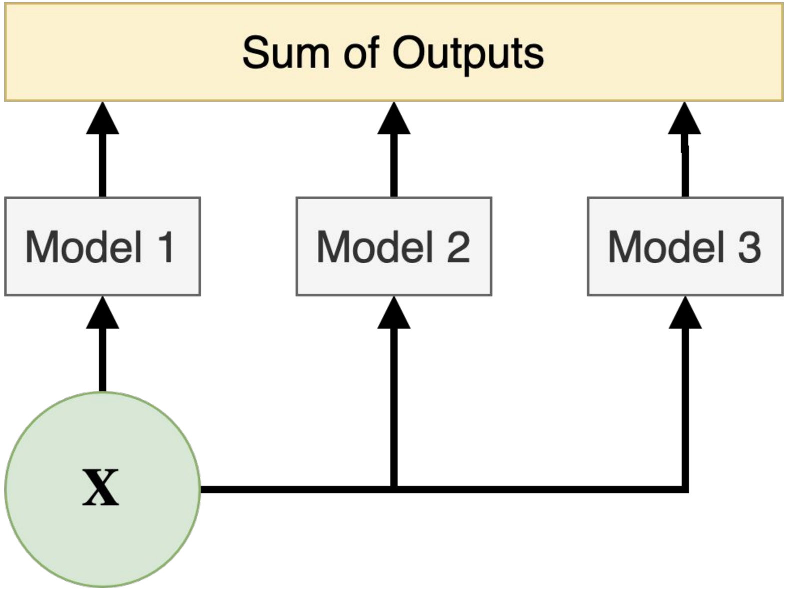
Sequential model training on the same dataset.

Each subsequent model is trained to output the residual of the previous model.



Gradient Boosting: Inference

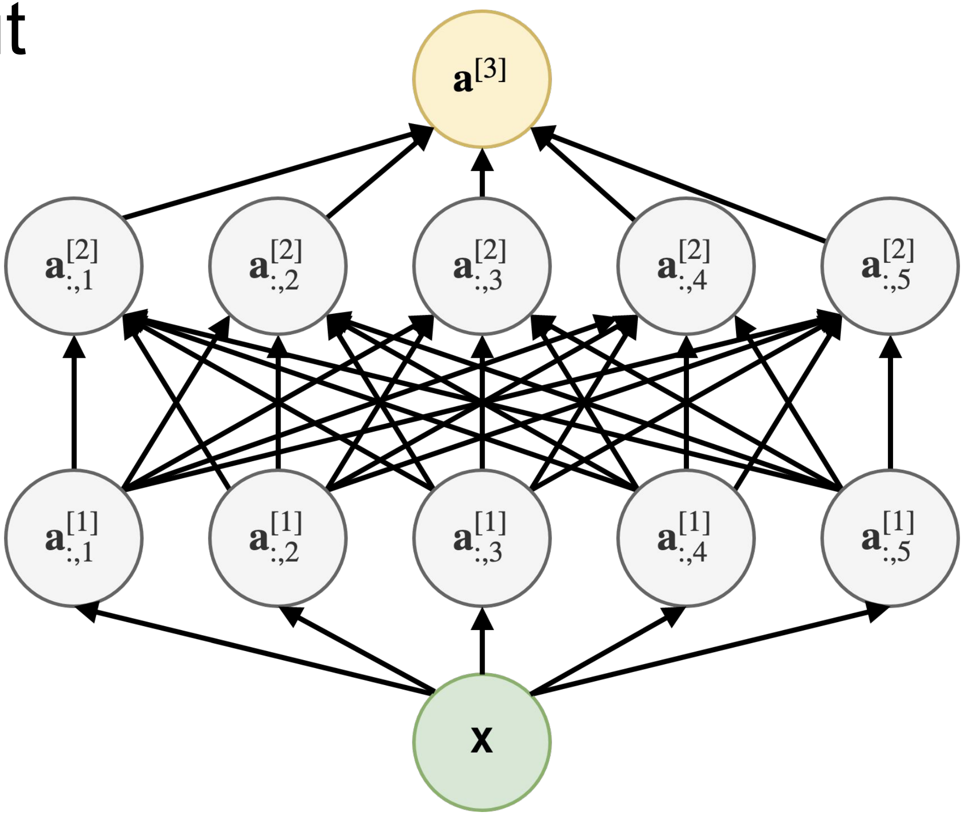
Ensemble output is the sum of outputs of each of the models.



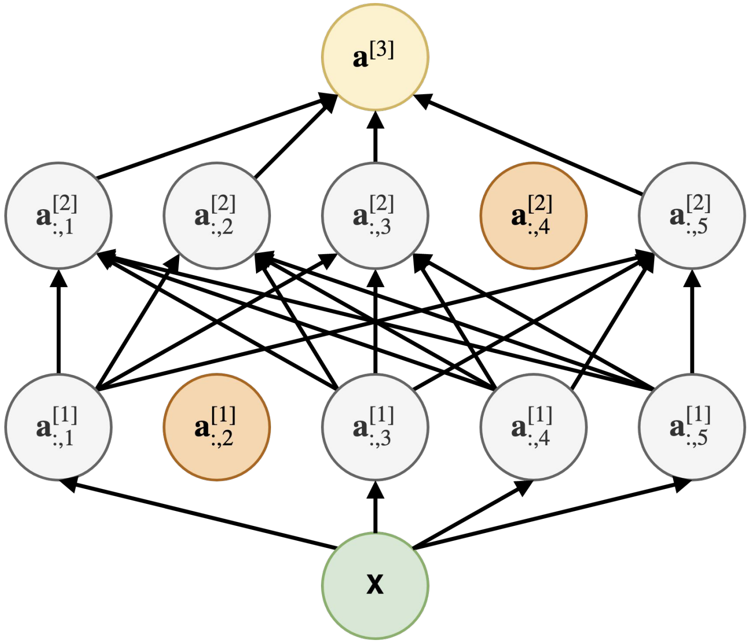
Noise Injection: Dropout

During training
On each iteration, randomly choose and disable nodes with fixed probability.

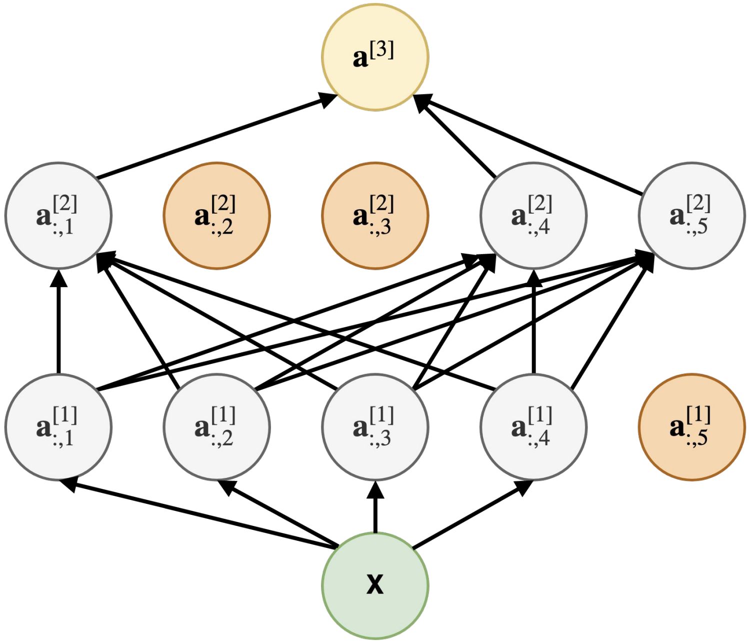
During inference
Use all nodes



Noise Injection: Dropout



Iteration 1



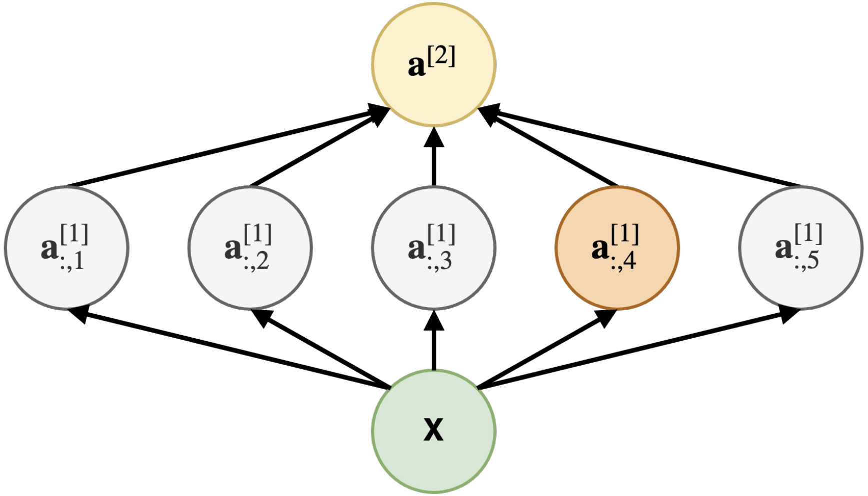
Iteration 2

Noise Injection: Dropout

Let's define:

- p = probability of keeping a node
- $\mathbf{d}$ = vector of random variables ~ Bernoulli(p)

$$\tilde{\mathbf{a}}^{[1]}_{:,m} = \frac{\mathbf{a}^{[1]}_{:,m} * d_m}{p}$$

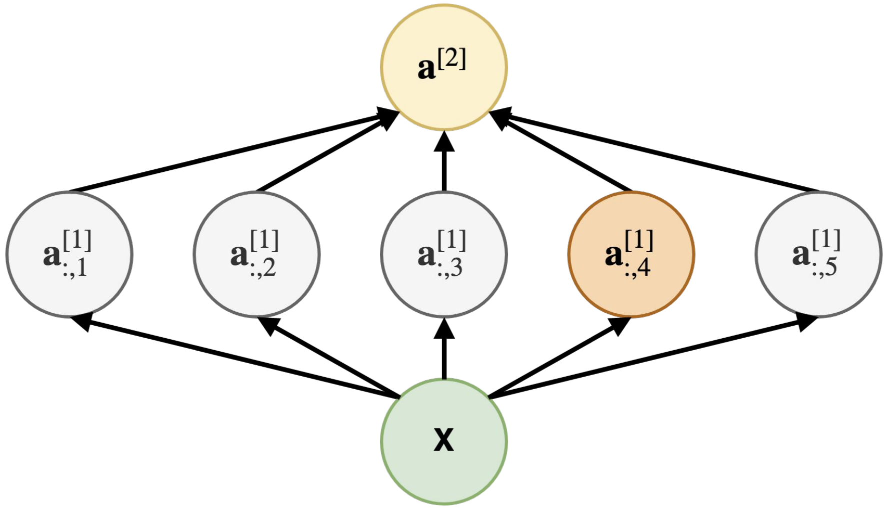


Srivastava, N, et al. (2014)

Noise Injection: Dropout

$$\tilde{\mathbf{a}}^{[1]}_{:,m} = \frac{\mathbf{a}^{[1]}_{:,m} * d_m}{p}$$

$$\begin{aligned}
\mathbb{E}[\tilde{\mathbf{a}}^{[1]}_{s,:}] &= \frac{\mathbb{E}[\mathbf{a}^{[1]}_{s,:}] * \mathbb{E}[\mathbf{d}]}{p} \\
&= \frac{\mathbb{E}[\mathbf{a}^{[1]}_{s,:}] * p}{p} \\
&= \mathbb{E}[\mathbf{a}^{[1]}_{s,:}]
\end{aligned}$$



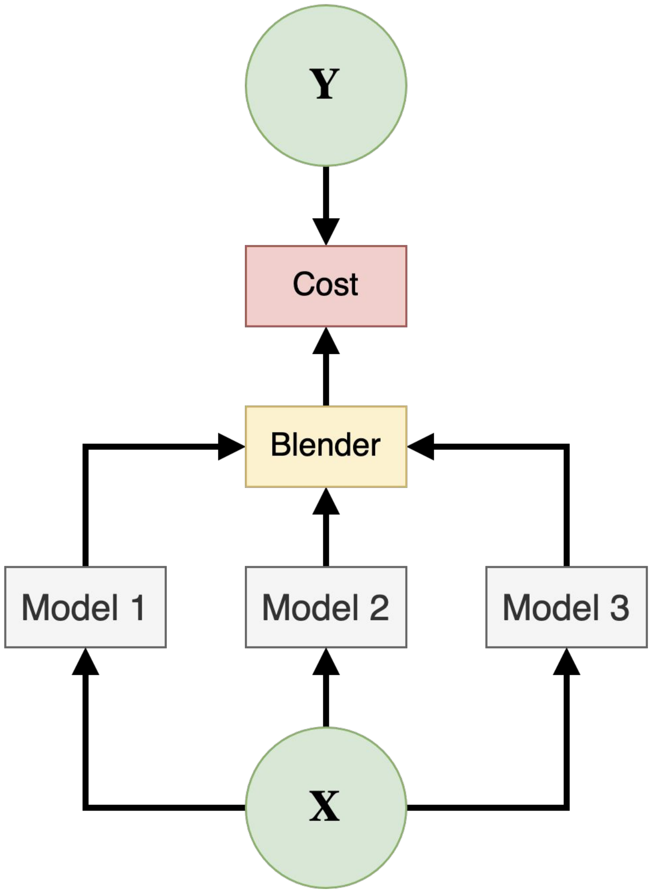
Srivastava, N, et al. (2014)

See Dropout.ipynb for discussion, and Keras implementations.

Stacking: Forward Pass

Instead of taking a simple average, the aggregation step can be an independent model taking outputs of ensemble members as input.

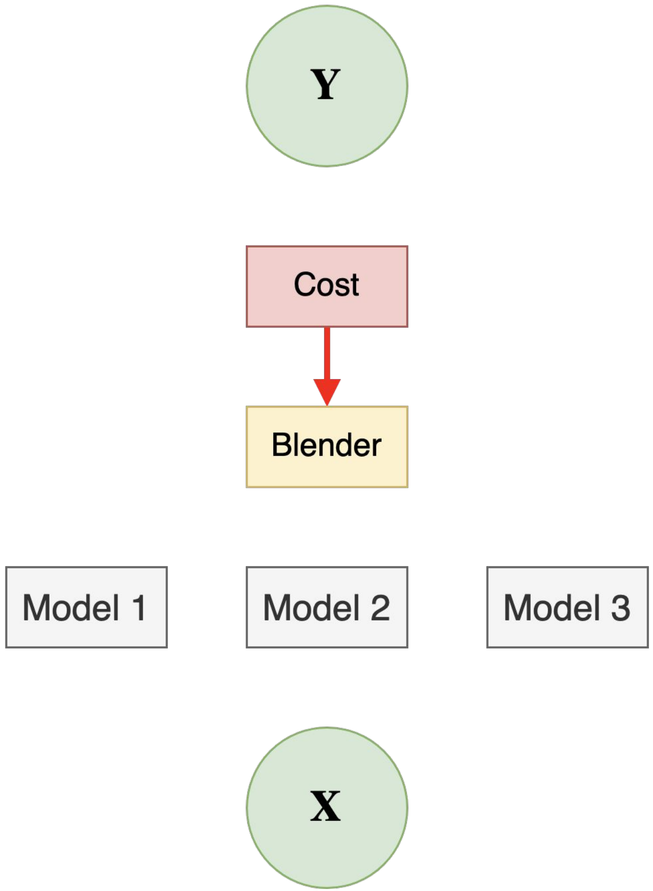
Blender is trained after the ensemble models have been trained.



Stacking: Backward Pass

Instead of taking a simple average, the aggregation step can be an independent model taking outputs of ensemble members as input.

Blender is trained after the ensemble models have been trained.



Examples from Previous Papers

Model	Diversity Source
GoogLeNet	Dropout + Batch seed
ResNet	Network depth
VGGNet	Dropout + Image size
AlexNet	Dropout + ?

Final Project

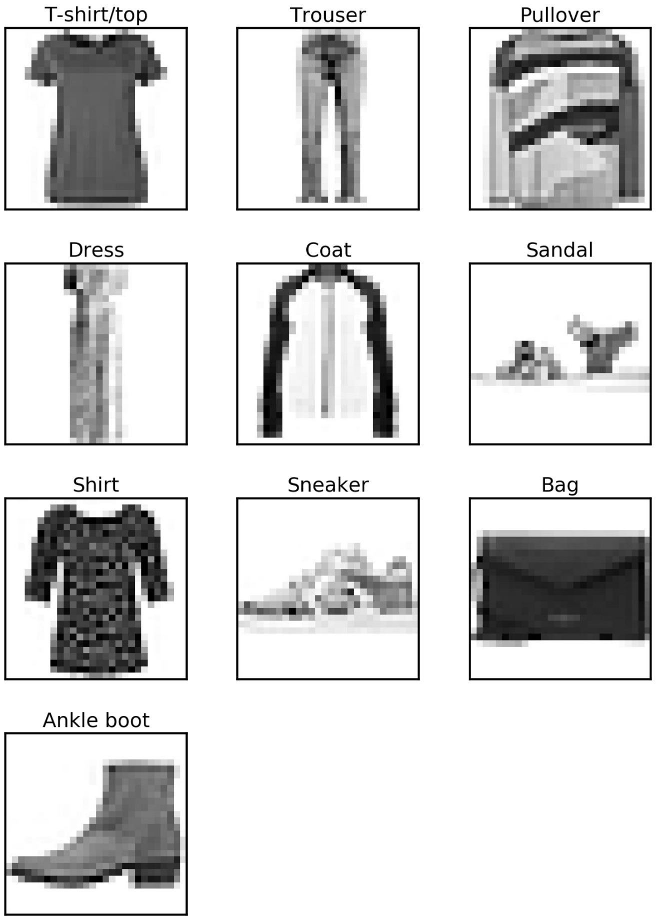
Dataset

70K images, 28x28 grayscale, 10 classes

Task

Image classification

Any neural network architecture, training procedure, preprocessing, and ensemble method.



Final Project

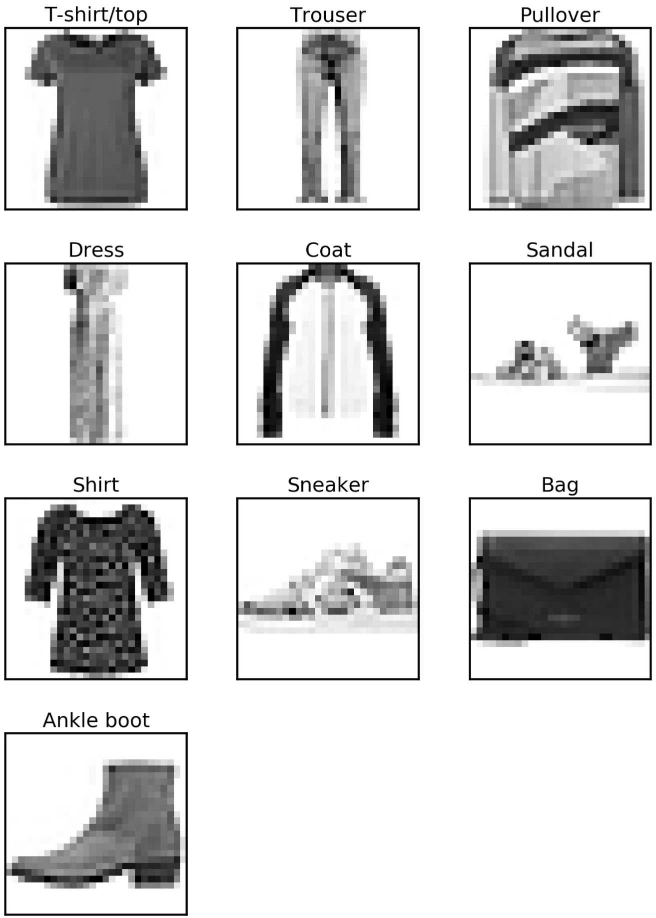
Grading

15 points = percentile of Log Loss

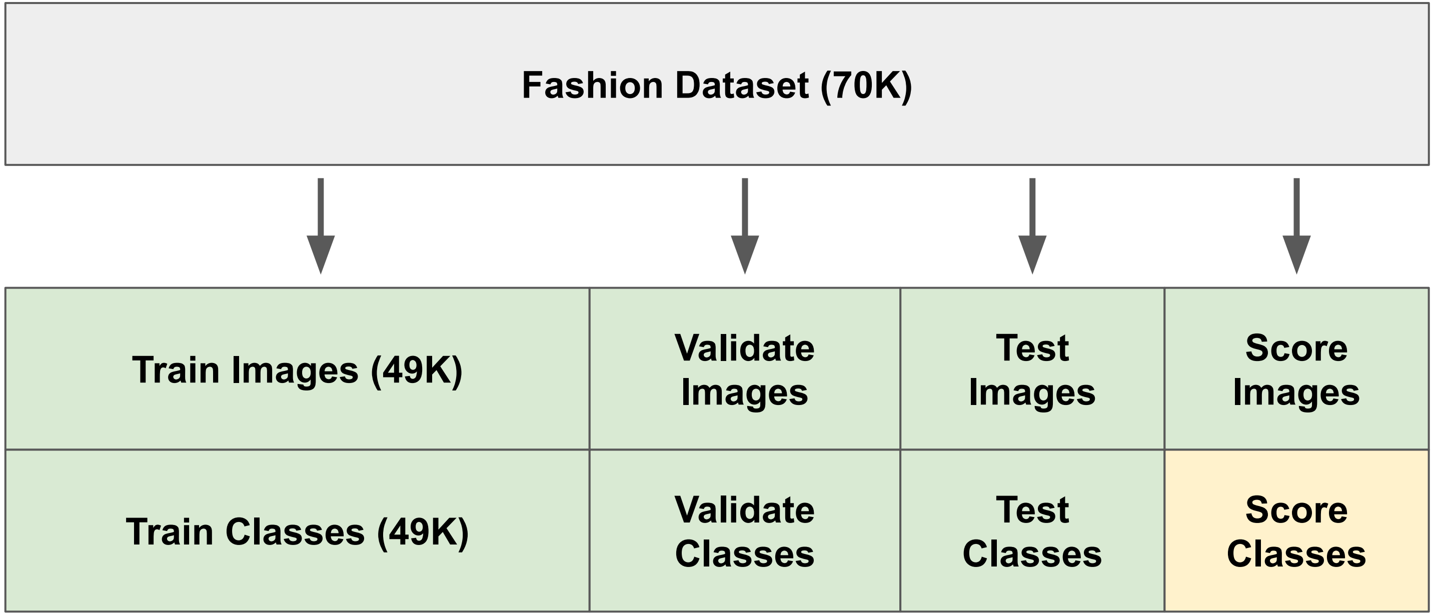
5 points = description of the solution

Deadline

EOD November 10th, 2020



Assignment Dataset



Demo

Assignment Template

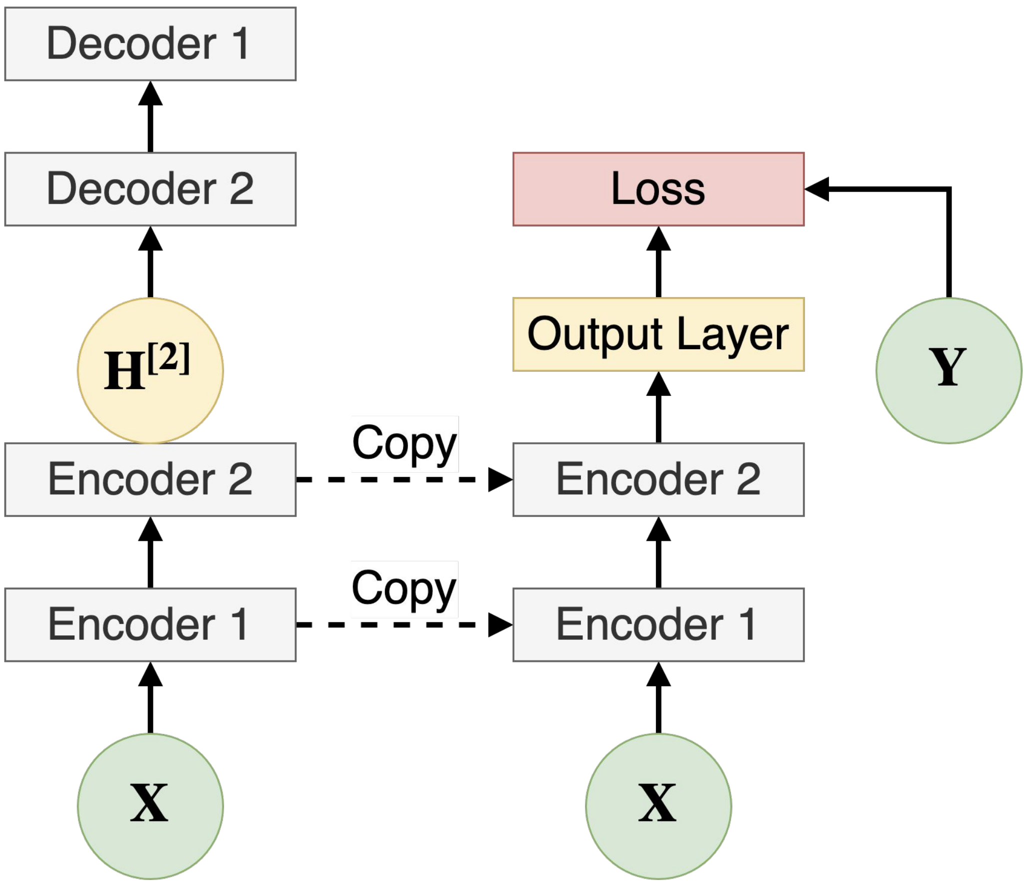
Demo

BigGAN Solution

Managerial Economics of Machine Learning

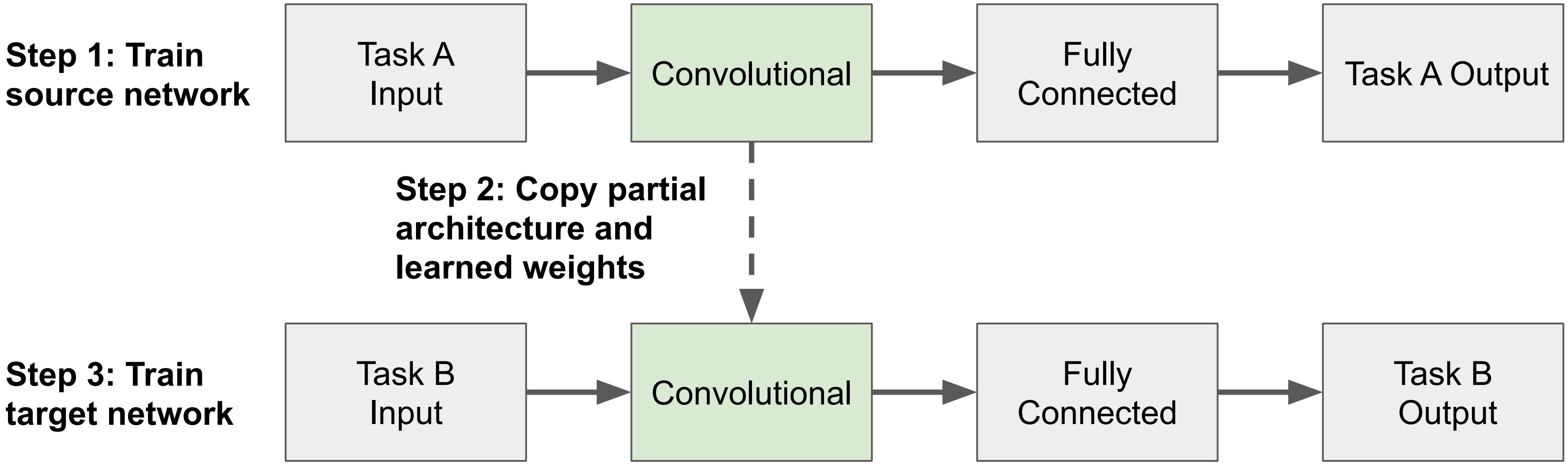
Project Goal	Project Duration	Training Cost	Required Training
Design new architecture and train from scratch	Months	Expensive	Machine Learning Researcher
Use pre-existing architecture and/or transfer learning	Weeks	Cheaper	Machine Learning Engineer
Find a pre-trained model and/or buy Inference as a Service API	Days	Free	Automation Software Engineer

Lecture 1: Unsupervised Pre-training



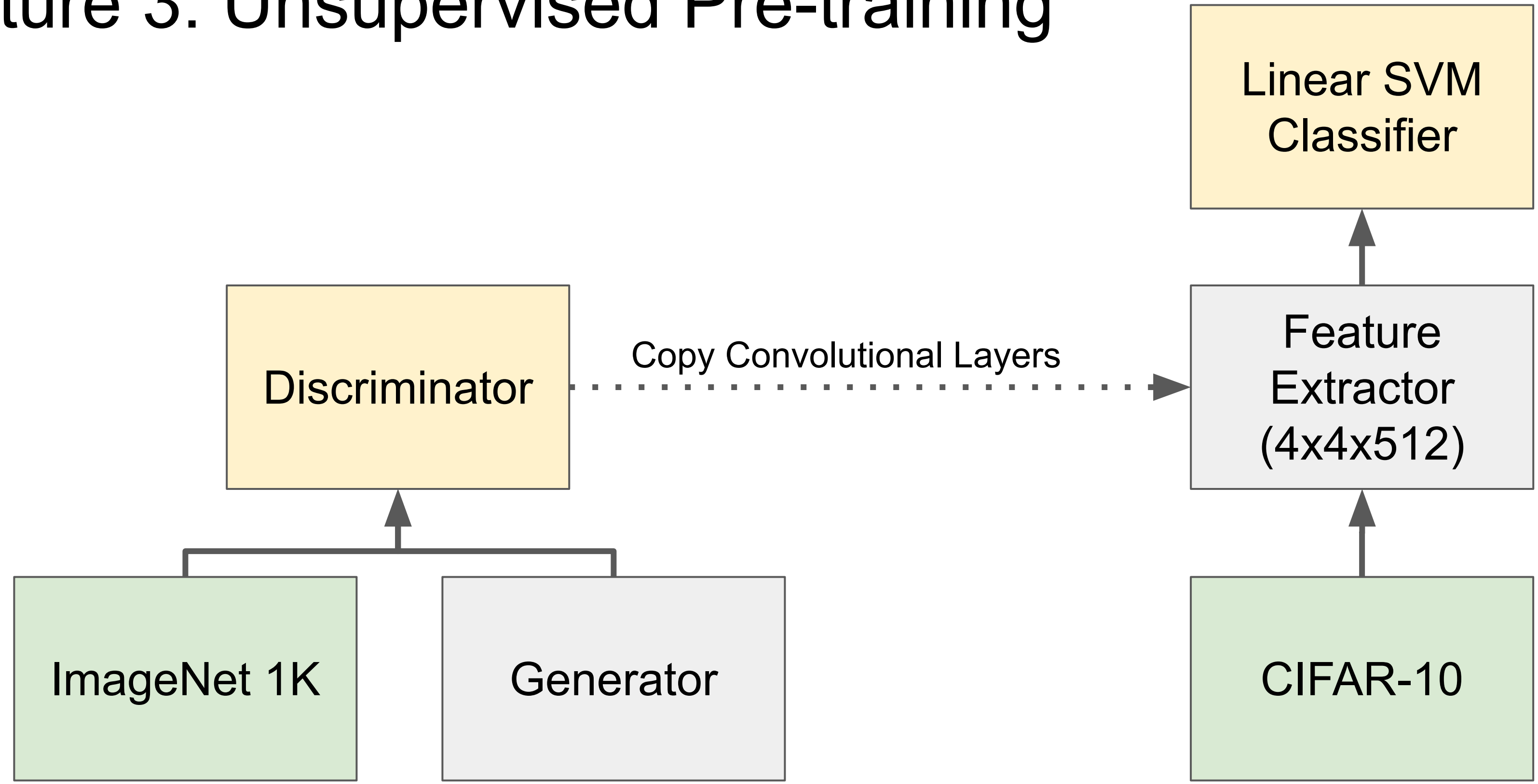
Bengio, Y., et al. (2007)

Lecture 2: Transfer of Supervised Learning



Tan, C., et al. (2018)

Lecture 3: Unsupervised Pre-training



Radford, A., et al. (2016)

AWS Rekognition

Product

~ $0.001 / image

Available as a convenient API

Features

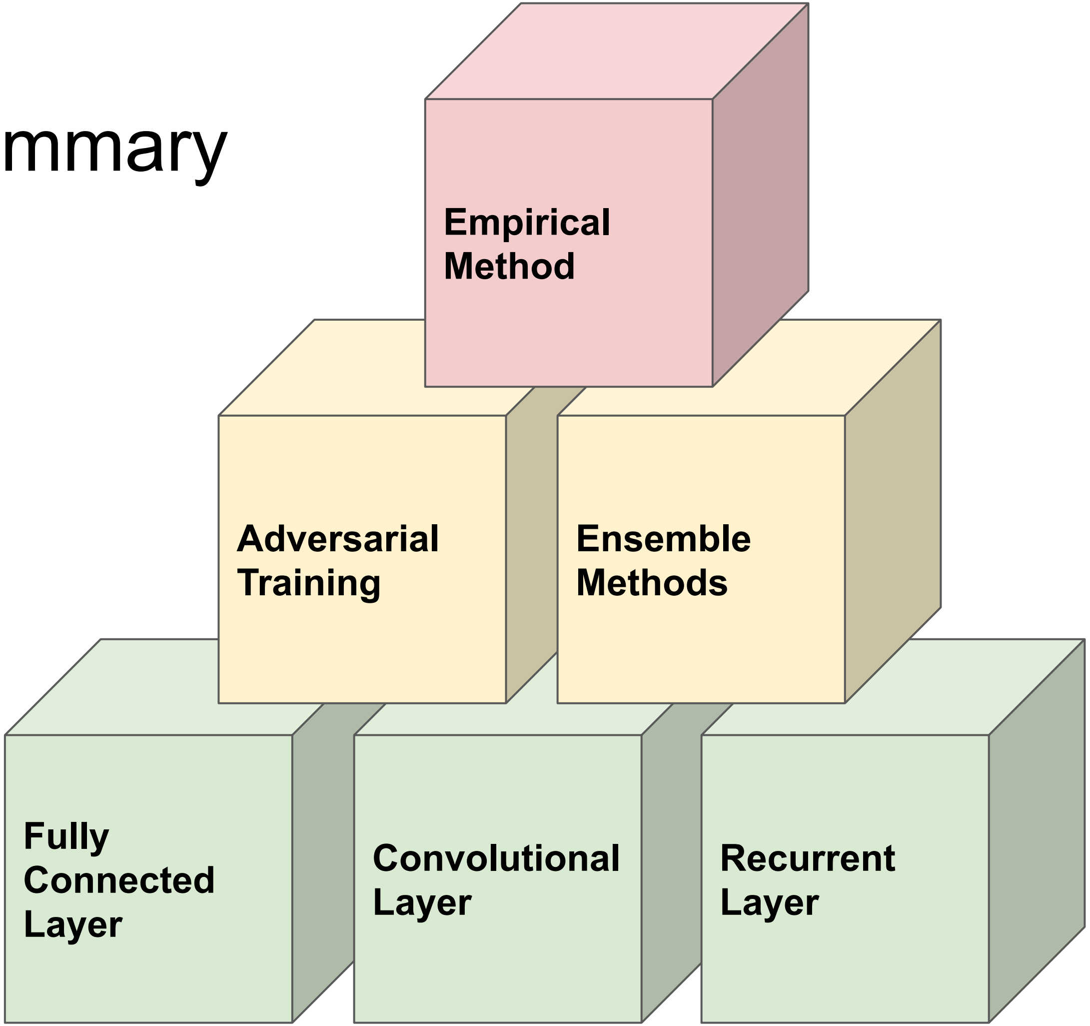
Object/scene detection

Face recognition and analysis

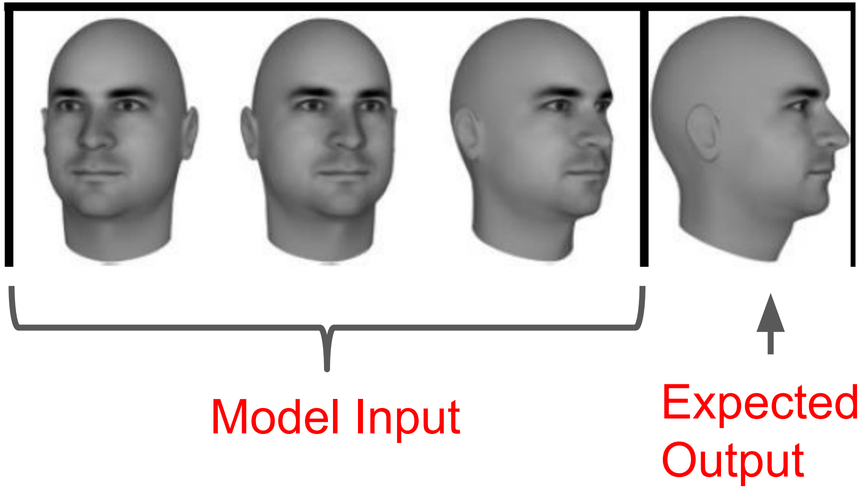
Both photo and video input

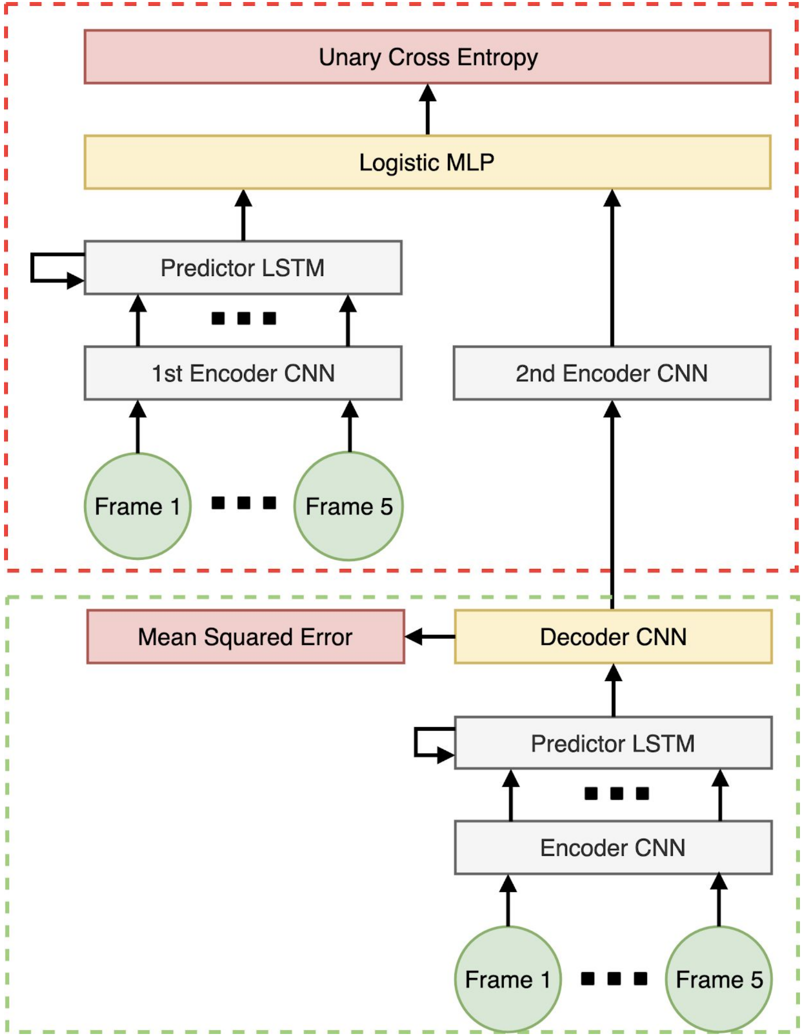
Image to text

Course Summary



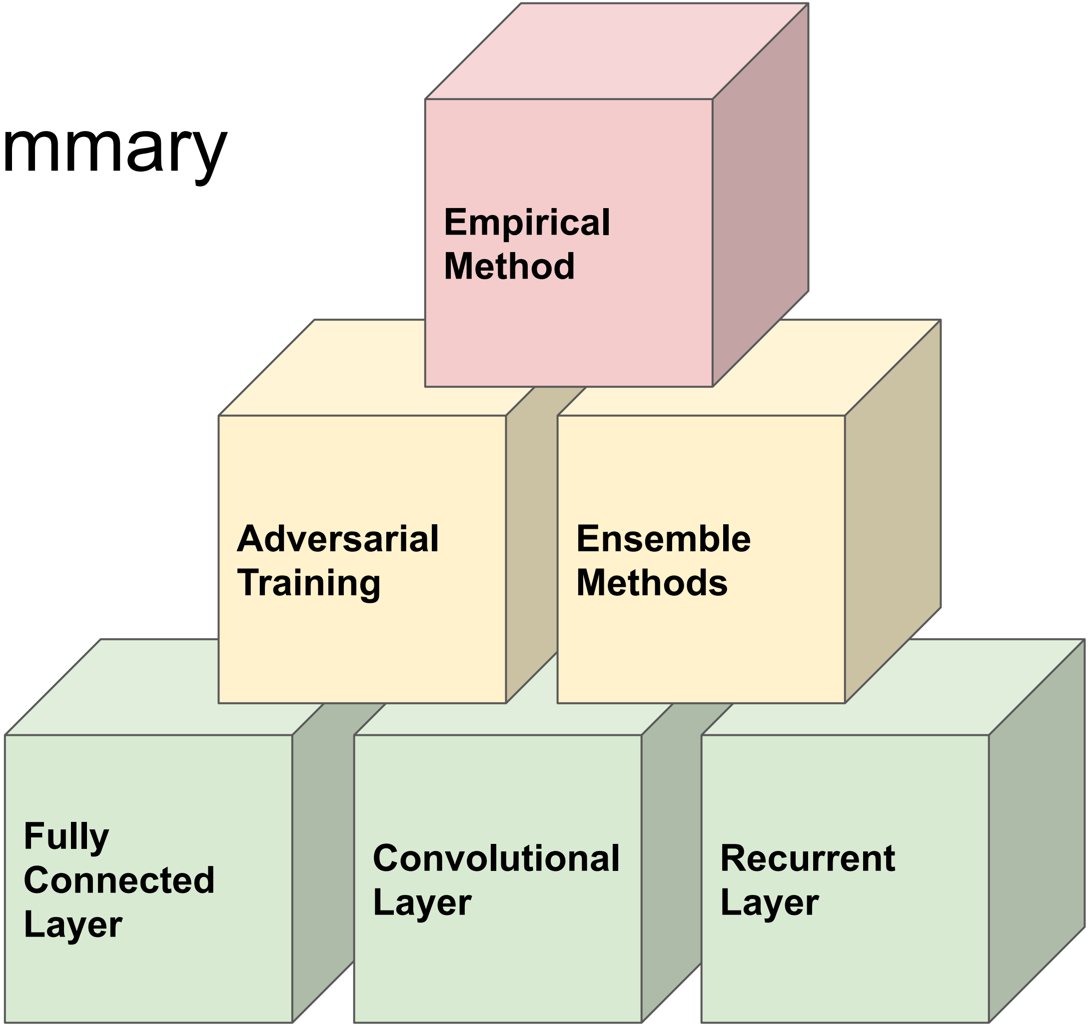
Lecture 4: PGN





Lotter, W., et al. (2016)

Course Summary



References

- A Short Introduction to Boosting (Fruend, Y., and Schapire, R. E., 1999)
- Dropout: A Simple Way to Prevent Neural Networks from Overfitting (Srivastava, N., et al., 2014)
- Ensemble Methods in Machine Learning (Diettrich, T. G., 2000)

Thank you

(Really) Final Q&A Time