

TBD Title

John Soper

A Thesis
Submitted in Partial Fulfillment of the
Requirements for the Degree of

Master of Science in Data Mining
Department of Mathematical Sciences

Central Connecticut State University
New Britain, Connecticut

Dec 2019
Thesis Committee:
Dr Zdravko Markov (Advisor)
Tbd1
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Abstract

Acknowledgements

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Introduction

Statement of Purpose

The objective of this thesis is in depth exploration of methods for classifying images with relatively small datasets (< 25k samples). Three datasets will be used, each with their own challenges:

1. Stanford Dog Breeds (fine-grained 120 classes, an ImageNet subset)
2. ImageNet_V2 Dog Breeds (same classes, but independent from ImageNet)
3. Flower Species (5 classes which are not represented in ImageNet)

The first section will discuss neural network theory starting from perceptron nodes. A simple, but comprehensive formulae set including forward- and backpropagation will be presented and analyzed. Deep learning definition, problems and abatement will be covered. A pure python coded neural network will be trained for XOR operation. CNN operation will be covered with analysis of how deep learning on images progresses in the order of edge detection, shape detection, lower-order features, higher-order features, and finishes with a one or more fully connected layer with softmax outputs.

The statistical makeup of the sample sets will be visualized, and any issues discussed. The V2 test data initially looks like it ill-conditioned with examples of both occlusion and conflicting classes (two or more in same image). It will be trimmed as necessary. The images will be used as is, but there will also be an augmented run which will include rotation, width and height shifts, shear and zoom range, and horizontal flipping.

The first procedure is to evaluate semi-advanced CNN trained from scratch. It contains five layers similar to VGG architecture but with just a single convolution per layer. Due to the small sample sizes, it is expected to perform only moderately and will provide a baseline for more advanced models. Captured metrics will include top-1 and top-5 accuracy (top-2 for flower data).

The second procedure which forms the bulk of this thesis will be experimenting with Transfer Learning on pretrained Keras application models, such as VGG, ResNet, and Inception. These have built-in weights from ImageNet and are quite powerful as is. Five activities are planned:

1. Classifying the 120 dog breeds directly and evaluating the false predictions ratio between non-dog and other-dog classes. Note there are 880 non-dog labels.
2. Simple bottleneck operation when the pretrained model without a top layer is grafted to a single softmax output layer sized to the number of expected classes. This is the most basic form of transfer learning.
3. Cascading two fully connected layers on the output and evaluating possible performance improvement from the ability to train more higher order features.
4. Fine tuning with the last CNN layer also allowed to train. To do this correctly, it must be after Step-2 bottleneck training so the weights in the last CNN layer train slower and correctly.

5. If step 4 results are positive, fine tuning of two or more CNN layers will be performed.
6. A stack of the three best models for possible performance boost.

The results from above will be visualized, analyzed, and discussed, especially in the context of Transfer Learning:

1. Alleviating the problems of small number of samples per class
2. Overfitting to the original ImageNet data
3. Adapting to completely different classes

Once the best single classifier or ensemble is identified, its misclassifications will be analyzed for root cause and possible improvements. There are many issues with fine-grained image detection which is why top-5 matches is a standard metric

After transfer learning, image classification using Mixup will be performed. This is a newer algorithm (Zhang, 2018) that embeds one image within another as a way to generalize and abate the effect of adversarial examples. It is founded on the idea that the features and class of a composite image can be considered a linear interpolation of its two source ones.

The final activity will be exploration of Contrastive Predictive Coding, an unsupervised algorithm for classifying images by training an image patch to predict another patch of itself. This involves training the neural network to learn a latent representation of the images. Once this is accomplished, a classifier can be formed by labeling a small subset of training images, which technically makes it semi-supervised learning, but different than the standard technique of imputing classes using similarity matrices.

DeepMind wrote the papers on CPC but did not release sample code. Therefore, the initial work will be done with the FashionMNIST dataset. This is 70k images of grayscale data with size 28x28 pixels. If results are successful, the code will be ported to the Flower dataset. Then there will make possible an interesting analysis and discussion of supervised versus unsupervised CNN learning on the same data.

Literature Review (3 parts)

1. General

The corpus of neural network (NN) technical papers is immense. One general overview (LeCun, 2015) discusses their advancement over time. An important benefit of NNs is that a hidden layer of perceptron nodes has the ability for representational learning of raw values. This is an improvement over other machine learning (ML) algorithms which may require complicated data transformations. The paper noted the invention of backpropagation by multiple groups in the 70s and 80s which allows multiple hidden layers and Deep Learning, the representation of data on multiple levels for in-depth processing.

NN popularity declined in the 1990s, then soared starting around 2006 due to larger datasets, more powerful computers, and the fact that high-dimensional cost function curves produce saddle-points instead of local minimums. The paper notes the success of supervised learning implemented with a variety of three major model families: Deep Feed Forward (DFF), Convolutional Neural Networks (CNN) and Recurrent Neural Networks (RNN). CNNs use sliding windows for input data which is large in one or more dimensions (typically 2D image pixels). RNNs generate output from the past output as well as current input and are usually preferred for sequential data such as time series or text. However, CNNs are sometimes used instead due to their versatility and ability for distributed training.

2. Transfer Learning

The large size of recent neural networks makes them quite powerful, but also difficult for the average user to train. A workaround is Transfer Learning (TL) which attaches a fully connected layer (or two) onto a pretrained NN (usually CNN-based) with some or all weights frozen. The new network can perform a more focused task with reduced data and training time.

(Pratt, Mostow, 1991) is one of the earliest papers on the subject. They applied a non-linearly separable dataset to a single hidden layer NN and observed the convergence results. The number of epochs needed with pretraining was about one third of that needed for random weight initialization. However, it would not converge at all about 20% of the time.

A survey paper (Pan, 2009) emphasized the point that TL is a minimal recalibration technique to make outdated training data (IE localized to a previous time or system) perform well on a newer target domain. The authors categorize the various implementations of TL as having three possible settings (inductive, transductive, and supervised), and four transfer contexts (instance, feature-representation, parameter, and relational-knowledge). The paper discusses current research issues concerning different source and target domains (or feature spaces). This reduces performance possibly to the point of negative transfer (worse than no transfer at all).

An additional TL paper (Bengio*, 2012), discussed how deep networks are like the human brain which forms higher-level abstractions as compositions of lower-level ones. And the lower-level ones can be useful for other domains which is what makes transfer learning feasible. The ideal learned features are abstract and disentangle all the factors of input variations.

(Yosinski, 2014) analyzed NN layers for image data in depth. The first layer learned features similar to Gabor filters and color blobs, and the second layer was also generalized. The paper measured the results implementing TL with frozen weights for layers after this and found two separate effects. Layers 3-5 dropped in performance due to lowered co-adaption (neurons in adjacent layers working together to resolve a feature). Layers 6-7 degradation was dominated by specificity to the original data and lack of generalization. The authors found that fine-tuning abated these issues, in some cases even outperforming a NN trained from scratch.

ImageNet performance was studied in detail (Huh, 2016) and it was found that commonly held beliefs are uncertain. In particular, they still achieved good TL results even when the pre-training used a reduced number of classes (127 vs 1000) or a reduced number of samples per class (500 vs 1000). They admit this phenomenon could be specific to the AlexNet architecture they used or possibly the PASCAL and SUN target datasets having similarities to ImageNet. They conclude by calling for more research to determine just how “data-hungry” CNNs really are.

A Google Brain paper (Kornblith, 2019) focused in depth on TL tradeoffs. They found that model accuracy on ImageNet data correlated to TL performance using a simple logistic regression (bottleneck) output layer. However, improving the ImageNet performance with regularization tended to drop TL accuracy. Implementing fine-tuning improved results and became less sensitive to regularization (but more sensitive to differences between datasets). Finally, fine-grained (many classes) data was examined for both TL and training from scratch. TL did not have higher accuracy but did have convergence times an order of magnitude less.

3. Unsupervised Learning

(Bengio, 2012) had this to say about unsupervised learning:

Although we have not focused on it in this Review, we expect unsupervised learning to become far more important in the longer term. Human and animal learning is largely unsupervised: we discover the structure of the world by observing it, not by being told the name of every object.

(Hinton 1986) is the first or nearly first mention of autoencoders, the oldest unsupervised NN model. They use a small hidden layer which act as a bottleneck to force a lower dimensional representation of the data. Their model in the chapter, not yet called an autoencoder, has an N-sized input layer followed by a $\log_2(N)$ -sized hidden layer which acts as a bit encoder after training.

(Mikolov 2013) discussed a groundbreaking algorithm called Word2Vec for creating word embeddings directly from unstructured text data. Its assignment of terms into 300-dimensional space was so accurate it even allowed vector math such as ‘woman’ + (‘king’ - ‘man’) = ‘queen’.

In the next year, Generative Adversarial Nets (Goodfellow 2014) were introduced. This is a very interesting algorithm: two neural networks (a generator and a discriminator) have opposite performance goals. Training is alternated between them with the weights frozen on the other. Each keeps supplying the other with more complex training data. The result is a GAN which models what the data looks like and can produce new samples on demand, i.e. density estimation.

(Radford, 2016) followed up the previous paper with improvements for unsupervised learning plus training stability. It discusses building GANs using simple convolution layers without max-pooling or fully connected layers. Once trained, parts of these DCGANs are used as feature extractors for supervised work, even to the point of image vector addition, similar to terms in Word2Vec.

Contrastive Predictive Coding (CPC) is a new unsupervised technique introduced in a DeepMind paper (Oord, 2019), and deals with extracting representations from unlabeled data. High dimensional data is encoded into latent space, then autoregression is used to summarize it into a context latent representation. For training, negative sampling is used to differentiate between downstream portions of the same distribution and different ones. The paper discussed the general theory and showed results in four different domains: speech, text, images, and reinforcement learning.

(Henaff, 2019) is a follow-up paper focusing on CPC for image data only. Its technique is to divide an image into overlapping patches each of which is encoded into a feature vector. Then feature vectors from a certain region (like the top half of an image) are aggregated with a context network into context vectors. A row of context vectors is then used to predict features vectors, in an unseen area (i.e. bottom half of the image).

Technical Overview

Neural networks are not new, but their popularity is. Perceptrons capable of the XOR function existed in the 70s, with backpropagation starting about 1975. However, the available datasets were small, and training either failed or took too long because of limited computer power. SVMs, Linear Classifiers, and Random Forests were more widely used, especially in the 1990s and early 2000s. In the words of Yann LeCun: “We were outcast a little bit in the broader machine learning community; we couldn’t get our papers published” (Allen, 2015).

Logistic Regression Nodes

Linear algebra is based on mappings which preserve addition and scalar multiplication in a system:

$$F(x_1 + cx_2) = F(x_1) + cF(x_2) \quad (1)$$

A linear regression node has multiple uses but cannot be the basis of a data processing network because any ensemble can only make a larger “linear sandwich” where the output directly scales from the input. In comparison, a logistic regression node runs the linear sum through a nonlinear activation function, typically the logistic function:

$$f(x) = \frac{1}{1 + e^{-x}} \quad (2)$$

The term *logistic regression* may seem like an incorrect name for a classifier, but the logistic function is continuous and bounded between 0 and 1. This is an example of a probabilistic classifier (Jaeger, 2003) where the output represents the probability of class membership. A simple decision rule, *max()*, makes it match other classifiers.

Perceptrons

A perceptron (aka neuron) is the building block of a neural network. It is basically a logistic regression node with a wider variety of activation functions but the same two input types:

- A constant bias value which effectively shifts the threshold point of the activation function left or right
- A weighted linear sum of inputs which is compared to the threshold to determine the pseudo-binary output value.

Single Perceptron Limitations

Even a non-linear activation function cannot meet all possible needs. For example, with the threshold set to 0.5, setting both inputs to a weight of 0.8 will produce the OR function, because either input is greater than the threshold by itself. However, weights of 0.4 will act like an AND function because both must be high to exceed the threshold. Multiple outputs can be created from a layer (column) of perceptrons, each performing AND and OR functions at different weighting. However, there is no way to perform the Exclusive-OR function with a single layer of perceptrons (Minsky, 1969).

Neural Networks

A neural network is a composition of perceptron nodes into multiple layers. The input layer will have one node for each feature, similarly the output layer will have one for each class. There will be one or more hidden layers in between to form intermediate products. With negative weighting acting as logical inversion, an exclusive-OR can be produced (Fig-1). Each node has a threshold of 0.5 and positive output of 1.0. The function of the single node in the hidden layer is to “kill” the output when both inputs are positive.

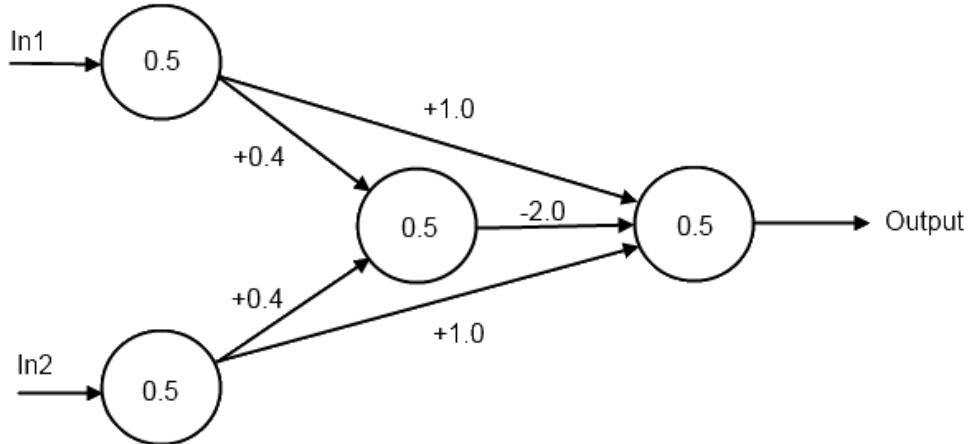


Fig 1: Hidden Layer Providing Exclusive-OR Operation

A classifier model to implement complex functions can be built from this foundation. In addition, neural networks can also perform regression by replacing the output layer activation with a simple identity function pass-through. Nonlinear regression is also possible from the contributions of multiple nodes in the hidden layer.

The creation of a functional neural network involves two interleaved steps, each using a dedicated labeled subset of the full data. Both are run through the model (forward propagation) to produce outputs which can be compared to the ground-truth labels. The first is training data which determines the correct node weights and biases through convergence. The goal is that the

model learns a general solution that also applies to unseen data. However, neural networks are very powerful and can memorize training set noise which is known as overfitting. Another point of view is that the hidden layers store a representation of the training data (Hinton, 2007).

The second step uses validation data to determine the correct hyperparameters (model conditions whose optimal settings are not obvious). Some examples are the number of hidden layers, their sizes, the learning rate, and the momentum value. The model is never trained on validation data, instead it acts as a substitute for unseen data. An *a-versus-b* type comparison is performed to determine which candidate performed better. This can be done in an ad-hoc manner under human control or a grid/random software search of multiple hyperparameter combinations (Claesen, 2015). Since validation performance improves with fitting but drops with overfitting, it is also used to trigger save points of model weights.

There are some variations of the above. Cross-validation is a time-sharing of training and validation data typically done with smaller datasets on other machine learning algorithms. There can also be a test data set which is only run at the end on the final model to determine if it is generalized. The reason for this is that a model can slowly become overfit to validation data when it is constantly adjusted based on it. A typical size balance between train/valid/test data is 60/20/20 percent for 10k points, but the last two can be shrunk as the data size grows because there is sufficient sampling of feature variance.

Neural networks are trained for a specified number of cycles through the entire training set known as epochs. Note: sometimes mini-epochs are used instead to decay the learning rate more frequently. An epoch is divided into segments based on batch size which is the number of samples run before updating weights. Modern computers support vectorization which performs vector operations with similar code statements and execution time as scalars. Since vectorization size is always a power of two, batch size should be also for an exact fit (32 is a good starting point).

Forward and Backpropagation

Training for both classifying and regression uses a cost function which is defined as a measure of difference between the predicted and ground truth distributions. It should be differentiable, always positive, and zero if the two distributions match. The first neural networks were more flexible and some even used a cost function based on genetic algorithms (Larose, 2005). However, backpropagation has superior performance and is now standard. This is also why neural networks use differentiable substitutes (i.e. logistic function for step function and softmax for max).

There are two reasons why differentiability is so critical for training neural nets. The first is gradient descent which minimizes a function by moving in the opposite direction of its gradient. Direct linear algebra solutions are ideal when possible (i.e. Ordinary Least Squares regression and Linear Discriminant Analysis), but gradient descent is a substitute when they are

not. Note: when gradient descent is also not possible, hill-climbing (shifting one feature at a time and retaining if improvement) can be used. The second related reason is that backpropagation needs it to compute the cost function with respect to all weights and biases using the chain rule. The chain rule formula states that the overall derivative for a composition formed with dependent variables is the product of their partial derivatives:

$$\frac{dz}{dx} = \frac{dz}{dy} * \frac{dy}{dx} \quad (3)$$

The complete back propagation algorithm of a NN can be formulated by applying four matrix equations derived from the chain rule. However, these equations are initially daunting and worse still, they are expressed in many different forms and notations across the literature. However, an intuitive version in vectorized form (Neilson, 2015) can be developed from the following schema (below and fig 2):

Z – weighted sums at a layer
 σ – nonlinear activation function
 a – output activations for a layer
 δ – error vector at point Z
 \odot – Hadamard (elementwise matrix) product

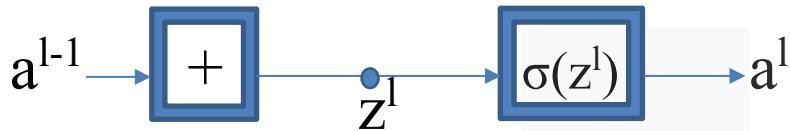


Figure 2: Basic Node Operation

Basic Feedforward NN Equations (for comparison)

Equations (4 & 5) specify forward operation. The output activations of the previous layer are linearly scaled with weights plus biases to form an input vector (z) which passes through a non-linear activation function (σ) to form activations which are the next layer's input.

$$Z^l = w^l a^{l-1} + b^l \quad (4)$$

$$a^l = \sigma(z^l) \quad (5)$$

First Equation: Error in Output Layer (L)

Backpropagation starts on the right at the output layer. The gradient (a vector of partial derivatives) is formed for the Cost function with respect to the output activations. Computing the Hadamard product (elementwise matrix multiplication) with the activation function's derivative effectively “steps back” the error to point Z^L in the output layer.

$$\delta^L = \nabla_a C \odot \sigma'(z^L) \quad (6)$$

Second Equation: Error in a Hidden Layer (l)

Similarly, repeated applications of the chain rule can step the error term backwards (leftwards) towards the preceding layers. Note: the layer weight column is transposed into a row for proper multiplication with the delta error column.

$$\delta^l = ((w^{l+1})^T \delta^{l+1}) \odot \sigma'(z^l) \quad (7)$$

Third Equation: Derivative of Cost with respect to Bias (b)

This equation is quite simple: in a given layer, the previously calculated error term is directly equal to the rate of change of cost relative to bias.

$$\frac{\partial C}{\partial b} = \delta \quad (8)$$

Fourth Equation: Derivative of Cost with respect to Weight (w)

The last equation ties it all together. The rate of cost change relative to a weight is the product of the activation with the error right at the weights themselves. This term is scaled by the learning rate (such as $\alpha = 0.01$) to compute a small value to shift the current weight value by. As the cost function approaches a minimum (local or global) in its multi-dimensional manifold, its derivative is reduced which produces a smaller weight shift as desired. Since the activation value is retained from forward propagation, the training process is a combination of chain rule and memoization. The rule of thumb is that backpropagation takes 3x the time of forward prop.

$$\frac{\partial C}{\partial w} = a_{in} \delta_{out} \quad (9)$$

Output Layer Activations and Cost Functions

In gradient descent, it is desirable that the update term shrink as the predictions become more correct. Expressing the delta error at the output layer's Z^L point as the predicted values minus the ground truth values works well. Since this point is reached through a single backpropagation operation, the delta is determined by an interaction between the derivatives for both the cost function and the output activation.

The solution is trivial when regressing because the activation function is an identity pass-through with a derivative of 1. A simple quadratic cost function suffices:

$$C(\text{reg}) = \frac{1}{2}(\hat{y} - y)^2 \quad (10)$$

Classification is more involved because the output activation is either the logistic function or its multinomial counterpart known as softmax. Both take the exponent of the Z^L value which produces a sigmoidal curve with flat sides. These areas of almost zero slope create difficulty for backpropagation, but cross-entropy cost functions provide a remedy:

$$C(\text{clf}_{\text{multinomial}}) = -\sum Y \log(\hat{Y}) \quad (11a)$$

$$C(\text{clf}_{\text{binary}}) = -y \log(\hat{y}) - (1 - y) \log(1 - \hat{y}) \quad (11b)$$

The multinomial formula (11a) is a sum over all output nodes (all possible classes), while the binary version (11b) is equivalent to having two output nodes that are always in opposite states. Cross-entropy is sometimes called log loss, a slightly different concept, which resolves to the same thing when used in this manner. The negative sign is needed because the log of a number between 0 and 1 will always be negative and a cost function should be positive. The main benefit of these equations is that the log operation inverts the exponential behavior of the activation. In fact, the delta term at Z^L is a simple subtraction just like for regression.

The TensorFlow and Keras deep learning libraries take things a step further and can perform softmax together with cross entropy in a provided API cost function routine. They claim the calculations are better for difficult corner cases. When using these, the output node activation will be set to an identity pass-through just like in regression. The term *logit* is often mentioned in the API documentation, which is the weighted sum (score) at Z^L that softmax turns into a probability.

Overfitting Abatement

As mentioned, neural networks are powerful enough to simply memorize their training data including its noise which hurts performance on unseen data. A large part of NN design focuses on avoiding this. There are three main categories of abatement methods: data, trimming, and tuning.

The simplest fix is to simply obtain more data. Noise is random and gets washed out with large populations. For datasets over a million samples, the validation and test sets can be a smaller percentage which increase the training data still more. For images, data augmentation is a way to effectively increase data. This involves operations such as shifts, flips, rotations, and skews. Some flips are harmful and should not be performed such as horizontal flips for numbers and vertical for horizons.

Trimming, the second category, reduces the possible solution space down to a subset which hopefully retains general solutions and discards overfit ones. Papers based on weight decay (Krogh, 1992) and weight sharing (Ullrich, 2017) have been published but the techniques have not become popular. In comparison, early stopping is supported in deep learning libraries and will save weights whenever a best validation score is reached. This hopefully takes a snapshot of the model at the sweet spot between fitting and overfitting.

Regularization is the most common trimming method and it penalizes the model for choosing a complex solution which usually indicates overfitting. L2 regularization adds the square of the weight value to the cost function of the corresponding node. Under these conditions, the algorithms will choose a more complex solution only when the cost reduction due to gradient descent is greater than the rise from the higher weight. L1 regularization is less common and simply adds the weight value to the cost function. During gradient descent, a constant value with the sign of the weight is present in the calculation. L1 and L2 have many other names and are seen in other models such as plain (non-NN) regression. They are sometimes cost functions themselves.

The final category is tuning, kind of a catch-all term. Dropout (Srivastava, 2014) made a huge impact and is widely used. It is the random temporary disconnect of connections between layers which forces the NN to learn alternate (more general) pathways. Dropout is only active during training and typically only on hidden layer connections. The size of hidden layers should correspondingly increased (i.e. 20% more nodes for 20% dropout). Also, the activation strengths need to be scaled to equalize the dropout and no-dropout conditions, but deep learning libraries automate this. Dropout roughly corresponds to bagging in random forests and has the same goal: to hurt the overfit more than the fit.

Another tuning method is normalization which is the scaling of values passing through a NN to avoid vanishing gradients, exploding gradients and dead RELUs. Before it was available, a more primitive technique called gradient clipping was sometimes used. A word of caution:

normalization is one of the most overloaded terms in machine learning and has other meanings depending on context:

1. Scaling a vector into a unit vector
2. Transforming a distribution to be more normal with the Box-Cox or Yeo-Johnson formulae
3. Standardizing data values to Z or min-max scales

Batch normalization (Ioffe, 2015) is the most commonly used flavor and calculates values for each location separately but using every sample in the minibatch. The formulae are similar to z-scores and perform scaling and shifting. Batch sizes should be as large as possible to minimize differences between them. This is usually the case anyway because of current large GPU sizes, but smaller batch sizes can produce a regularization benefit with noise, so batch size is another machine learning tradeoff. Since RNNs take past outputs as inputs, batch normalization is very difficult and layer normalization is typically preferred. It performs calculations on a single sample at a time but using all values in a given layer. There are other normalizations available that are seldom used. Batch normalization has become very popular similar to dropout and is sometimes preferred over it. The dropout rate should be reduced if both are used together.

The last common tuning method is transfer learning which will later be covered in depth.

Remaining Topics

The current state of deep learning has moved beyond logistic activations and they are typically now seen only in the output node for binary classification. Rectified Linear Units (ReLUs) have become the current standard. They act as an identity function ($y=x$) for positive inputs and output 0 for negative ones. The right-sided derivative of 1 minimizes the problems of vanishing and exploding gradients. They can still occur, but only through an unlucky concatenation of weights. Since the slope at $x=0$ is discontinuous, the ReLU function is not differentiable, but this is not a problem. Each half is handled separately which is formally known as subgradient descent.

Other activations and their derivatives are shown in Appendix-B. Tanh is a shifted and sharper version of Logistic, while Leaky ReLU gives dead ReLUs (negative input) a backpropagation pathway to possibly turn back on.

Momentum is a term added to the cost function to fix a geometric issue. A gradient descent point may become stuck in a valley bouncing between walls with slow progress towards the exit. Momentum adds a decaying sum term to the weight update which increases the common component (moving out of the valley) while reducing the differential one (alternating directions towards valley walls).

A variation is Nesterov Accelerated Gradient which adds the momentum vector to the new weights instead of including it in their calculation.

Gradient descent optimizers (Duchi, 2010) were another leap forward in NN design. They allow parameters to have individual learning rates instead of a single global one. The most frequently occurring features have smaller updates and infrequent ones get large ones. In addition, the learning rate no longer needs tuning, the default value works well in most cases. Adagrad was one of the first implementations, it scales the learning rate by a reciprocal root-sum-square term of decaying past gradients. Adadelta is similar but the number of past gradients gets capped at a set window size. Adaptive Moment Estimation (Adam) (Kingma, 2015) is basically Adadelta with decaying past momentums included. It is good at all-around performer and used in many projects.

Finally, the initial values for weights in deep learning have evolved over time. The mean value is still 0.0 in all cases, but different variances can be used based on the activation function and both fan-in (N_i) and fan-out (N_o) with bordering layers (Eq 12a-d). Curiously, the Keras documentation recommends a truncated normal initialization with a stddev of 0.5.

$$Var(primitive) = 0.1 \quad (12a)$$

$$Var(LeCun) = \frac{1}{N_i} \quad (12b)$$

$$Var(He) = \frac{2}{N_i} \quad (12c)$$

$$Var(Xavier \text{ aka Glorot}) = \frac{2}{N_i + N_o} \quad (12d)$$

Basic Update Equations

Tying together the above information, the basic update formulae for weight and bias updates in gradient descent are:

$$W_{t+1} = W_t - \frac{\eta}{m} \sum (A^{l-1}) \delta^l + uv_W + \eta\lambda W_t \quad (13)$$

$$B_{t+1} = B_t - \frac{k\eta}{m} \sum \delta^l + uv_B \quad (14)$$

Where:

η = learning rate

m = batch size (which sigma sums over)

u = momentum coefficient (0 if not used)

v = current momentum

λ = L2 coefficient (0 if not used)

k = fudge factor because some libraries update bias at a different rate than weights

Debugging Tip

When designing a neural network classifier, it helps to first verify basic operation with a tiny data subset such as 32 samples (16 samples each of two classes). It is used for both training and validation with a batch size also 32. The model should easily memorize the data and overfit to an accuracy of 100% while the cross-entropy cost function drops from nearly 1 to 0. This will not catch every issue but is a quick way to detect the “low-hanging fruit”.

Simple Python Neural Network

As a demonstration, a primitive NN was coded up in Python using Numpy arrays and trained for the XOR function (code in Appendix-B). For simplicity, there were no biases, a simple passthrough was used for the output activation, and the cost function was quadratic. The training converged (Fig 3) and the output is high only for inputs (0, 1) and (1,0) which is proper XOR operation function.

Epoch	Loss	Y(0,0)	Y(0,1)	Y(1,0)	Y(1,1)
0	4.47936	0.0000	0.2773	3.7598	0.9054
100	0.54947	0.0000	0.3644	1.8336	0.0000
200	0.21144	0.0000	0.4612	1.3640	0.0000
300	0.11149	0.0000	0.5610	1.1738	0.0000
400	0.06285	0.0000	0.6561	1.0860	0.0000
500	0.03471	0.0000	0.7401	1.0432	0.0000
600	0.01837	0.0000	0.8096	1.0219	0.0000
700	0.00932	0.0000	0.8639	1.0111	0.0000
800	0.00457	0.0000	0.9046	1.0057	0.0000
900	0.00218	0.0000	0.9340	1.0029	0.0000
1000	0.00102	0.0000	0.9548	1.0015	0.0000
1100	0.00047	0.0000	0.9693	1.0008	0.0000
1200	0.00022	0.0000	0.9792	1.0004	0.0000
1300	0.00010	0.0000	0.9860	1.0002	0.0000
1400	0.00004	0.0000	0.9906	1.0001	0.0000
1500	0.00002	0.0000	0.9937	1.0001	0.0000
1600	0.00001	0.0000	0.9957	1.0000	0.0000
1700	0.00000	0.0000	0.9971	1.0000	0.0000
1800	0.00000	0.0000	0.9981	1.0000	0.0000
1900	0.00000	0.0000	0.9987	1.0000	0.0000
2000	0.00000	0.0000	0.9991	1.0000	0.0000


```
final h_weights:  
[[ -0.41675785 -0.05626683 -2.1361961  0.57535004]  
 [-1.79343559 -0.84174737  0.98685426 -1.29664876]]  
  
final y_weights:  
[[ -1.05795222]  
 [-0.90900761]  
 [ 1.0124547 ]  
 [ 1.7380754 ]]
```

Fig-3: Metrics of Python Neural Network Training

Convolutional Neural Networks

CNNs are designed for data which is large in one or more dimensions, typically images. When convolving a grayscale image, a small 2d matrix known as a filter (aka feature detector) traverses the image as a sliding window, computing dot products at each step, which builds up a feature map. Multiple filters can be trained to detect different features and produce a set of feature maps. Each feature map can also be pooled (aka subsampled) into a smaller one. Therefore, data traveling through a CNN tends to shrink in two dimensions and grow in the third. The final layer is fully connected and produces softmax class predictions in the usual way (Fig-4).

CNNs have a couple of big advantages which makes them a popular workhorse in deep learning. The first is that the sliding windows can process larger dimensional data than a fully connected layer could handle. A basic example is a 1000x1000 image that would require a million FC input nodes. Secondly, the adjacent feature maps are independent so they can be processed in parallel on multiple cores, a feature which RNNs sorely lack. Simply put, there is nothing better than CNNs for image processing.

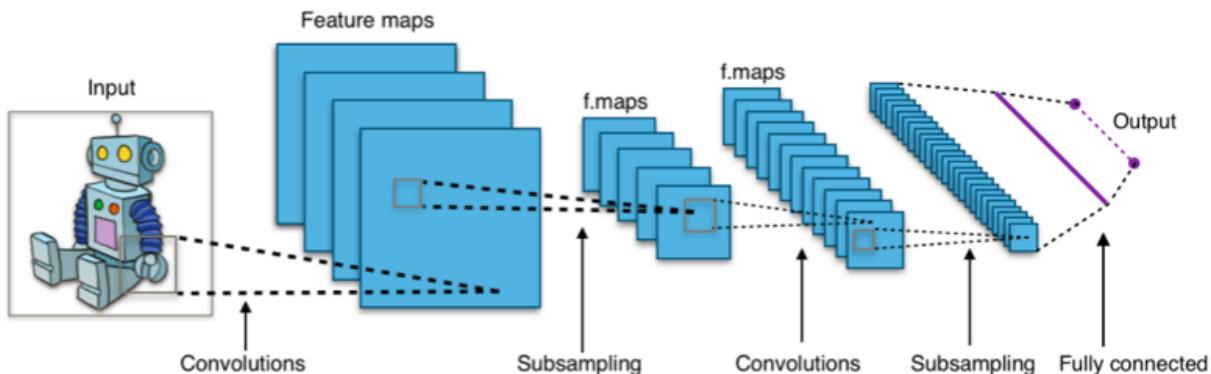


Fig-4: Basic CNN Structure (by Aphex34 - Own work, CC BY-SA 4.0),
<https://commons.wikimedia.org/w/index.php?curid=45679374>

Once CNNs are understood at a higher level, several complex aspects remain. Firstly, the filter x- and y-axis size (aka receptive field) are hyper-parameters, but the depth must match the preceding layer. Unlike grayscale images, color ones have a z-axis depth such as 3 (RGB) or 4 (CMYK) which locks in the depth of the first filter. The generated feature map is still 2D, but there can be more than one of them (another hyperparameter). If a CNN is trained to distinguish colors, it will carry the color information through all feature maps. However, if it is instead trained for character recognition, it will basically convert the image to grayscale internally since a red *B* and a blue *B* are the same class.

The filter interacts with several size settings due to its sliding window nature. The number of pixels it steps across is called stride. The image may be edge-padded with zeros to preserve the input size or to ensure the edges interact with the center of the filter matrix. The formula for output size along the x or y axis is:

$$O = \frac{I - W + 2P}{S} + 1 \quad (15)$$

where:

O = output feature map size

I = input feature map size

W = filter size

P = padding per side

S = stride

If the stride is one and the padding set to $P=(W-1)/2$, the x and y dimensions stay constant. However, a stride of two or more will reduce dimensions. Often the filter size is odd to process a single pixel with respect to its neighbors. An example of this is edge detection which is the first layer when processing images. From fig-5 below, the convolution dot product is set to produce large values when the center pixel is a different brightness from its surroundings.

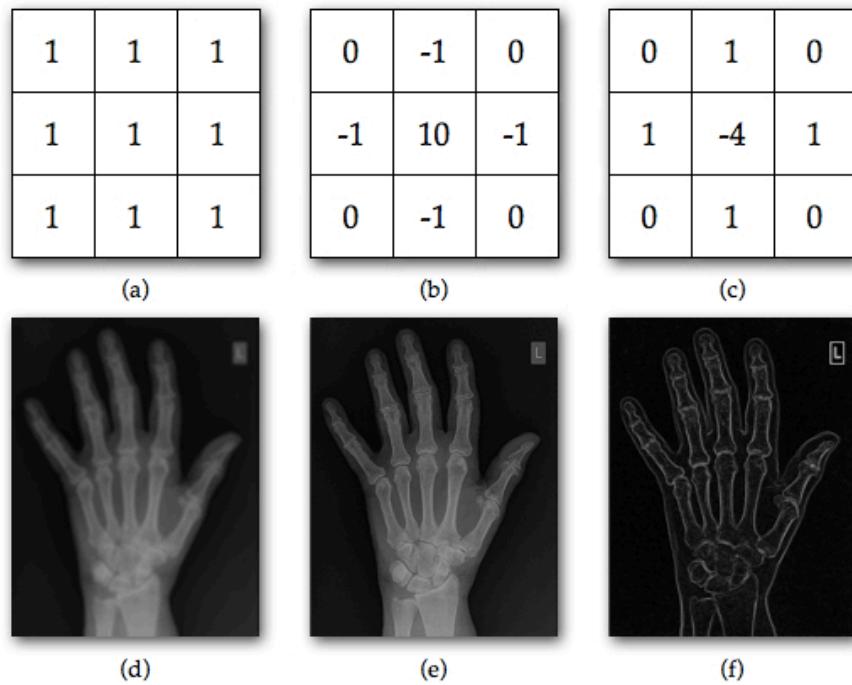


Fig-5: Edge Detection Filters (By Kieranmaher - Own work, Public Domain)
<https://commons.wikimedia.org/w/index.php?curid=13305900>

The pooling layer is another confusing part of CNNs because it has its own filters and stride. They are usually set identically, so that values appear only once. A max operation is standard (fig 6), but sometimes averaging is chosen instead. Not every convolution layer has a pooling layer after it and some people advocate against them (Springenberg, 2015). Therefore, a CNN has two ways to reduce dimensions: convolving with a 2+ stride and pooling. Both are optional, but a design without either one would be nonsensical.

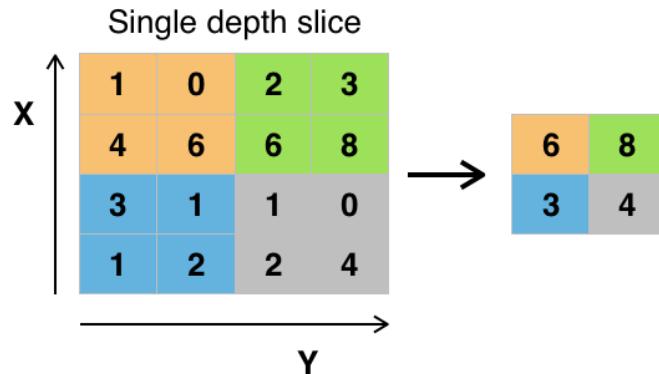


Fig-6: Simple Max-Pooling Example (By Aphex34 - Own work, CC BY-SA 4.0)
<https://commons.wikimedia.org/w/index.php?curid=45673581>

The last aspect of CNNs to understand is that they are still neural networks with weights, training, and backpropagation, just without full connections. The CNN filter is not a literal sliding window, that is just an abstraction to understand the process. Instead there is a stack of filters with identical weights, one for each possible convolution position, and each one of those connects to one position in the previous feature map. Adjacent feature maps in the next layer will have their own filter stacks with the same dimensions but different weights feeding them.

Backpropagation is performed by rotating the filter 180 degrees and performing convolution from back to front. Filters and fully connected nodes are trained while pools and ReLU (if used) are constant.

A numeric example for one layer is taken from the 2012 ImageNet Challenge winner (Krizhevsky, 2012):

- Image size = $224 * 224 * 3$ layers
- Filter size $11 \times 11 \times 3$ with stride 4 and double-sided padding of 3
- Output dimension = $(224 - 11 + 3) / 4 + 1 = 55$
- K = 96 feature maps
- Output volume = $55 \times 55 \times 96$
- Unique weights = $11 \times 11 \times 3 \times 96 = 34848$
- Unique biases = 96

Data Description and Preparation

Flower Dataset

Three image sets were used for this thesis (links in Appendix C). The first is a Kaggle dataset of 4328 images over five flower species. The files are in jpeg format with various sizes from about 150 to 300 (sometimes up to 600) pixels per axis. About 80% are landscape format the rest square or portrait. They were split into 70% test, 30% validation, stratified for class (Table-1):

Table-1: Flower Dataset

Species	Train samples	Valid. samples	Total Samples	Example 1	Example 2	Adversarial Example
Daisy	538	232	770			
Dandelion	736	317	1053			
Rose	549	236	785			
Sunflower	514	221	735			
Tulip	689	296	985			
Total	3026	1302	4328			

Flower Data Analysis

The images are well lit and almost always in focus. Some photos show additional content such as a vase or human, but not occluding the flower, except for an occasional insect in closeups. The images are a mix of single and multiple flowers. Most flowers are in bloom, some are buds or budding. Additionally, many of the dandelion images are seed pods (what children blow on). They appear different enough to be a sixth class which may explain why dandelion images have the largest representation (1053 images). Less than one percent of the samples look like an adversarial example, but some of them are very unfair.

A person must think in terms of shape and color to predict how a CNN might train on an image set. With flowers, the shape of the top parts (petals and pistils/stamens) will be the main differentiator between classes. For both top-down and level views, this will be a circular or oval shape, so the CNN layers after edge detection should train to recognize it.

Color is a mixed bag and the occasional black and white images do not help. Daisies (white petals around yellow center) and sunflowers (yellow petals around orange-brown center) will probably benefit the most from color information. Dandelions have two modes (solid yellow petals and white seed pods) but at least those colorings are constant. Roses and Tulips are known for having many colors however, and the CNN will have to focus more on shapes. Green from the surrounding vegetation and blue horizons from sky are worthless for class differentiation and will probably not be learned.

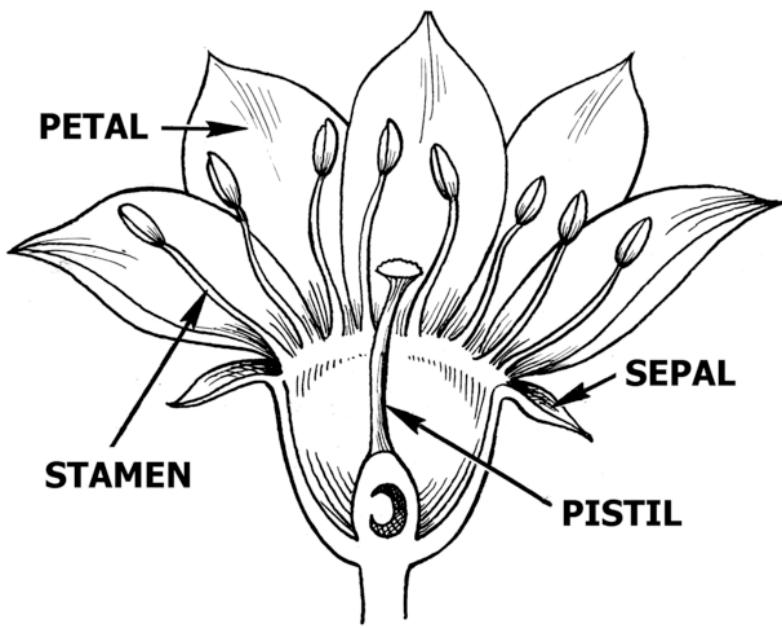


Fig 7: Flower Anatomy (Public domain)
[https://commons.wikimedia.org/wiki/File:Flower_Anatomy_\(PSF\).png](https://commons.wikimedia.org/wiki/File:Flower_Anatomy_(PSF).png)

Stanford Dog Breed Dataset

This set is composed of 20,580 images across 120 dog breed classes and is intended for fine-grained classification. This is a branch of object recognition where the different classes share generic features and the model must be trained for additional aspects. The files are in jpeg format with slightly over two thirds in landscape mode. The average number of pixels per axis is higher than the Flower data usually in the 300-500 range.

The number of samples per class ranges from 148 for Redbone to 252 for Maltese_dog (full breakdown in Appendix D). For this study, the data was split for a constant 30 validation and 20 test samples per class. Therefore, the number of training samples for a class is 50 less than the total samples. Five breeds were sampled by taking the first and last ones alphabetically (Table-2). Differentiating between the two terrier breeds is an example of challenges the models will face.

Table-2: Stanford Breeds (PARTIAL)

Species	Total Samples	Example 1	Example 2	Adversarial Example
Affenpinscher	150			
Afghan Hound	239			
African Hunting Dog	169			
Wire-haired Fox Terrier	157			
Yorkshire Terrier	164			

Stanford Dog Breed Data Analysis

The images are similar to the Flower dataset in terms of being in focus, good lighting and hardly any occlusions. Most photos are of a single dog, a few have two or more of the same breed, and one adversarial example with two breeds was noticed. The settings were more varied than the flowers and included indoor scenes and even dog shows. There are more images with humans present, but still relatively few. Dog colors are subdued and will a less important feature than the bright hues of flowers.

The American Kennel Society (AKC) recognizes seven groups of dog breeds: Terrier, Toy, Working, Sporting, Hound, Non-Sporting, and Herder. Some of their characteristics will be learned by a classifier. Hounds tend to have pointed ears to hear prey and long legs to chase it down. Toy dogs have curled tails and relatively large eyes which reflect their status as cute indoor pets. Breeds known for fighting usually have large necks and full muscles for protection. Dog breeds are different sizes as well (from small toy breeds to large hounds) but photos have no sizing scale reference to supply the neural network.

There are two big drawbacks to classifying this dataset balanced by one large advantage. The first issue will be all the possible dog orientations. Some photos are frontal, some sideview, but most are in between. There are also varying degrees of downward angle because of cameras being at the level of human eyes. The neural network will have to detect the dog's head from different perspectives with its body supplying additional features.

The second problem is that fine-grained classification of 120 different targets is a lot to expect from a model. Dog breeds make this harder still because some have very similar appearances such as Malamute & Siberian Huskey or Italian Greyhound and Whippet (Fig-8). For this reason, papers about image classification also report if the correct class is in the top five predictions. One interesting piece of trivia is that dalmatians were left out of the dataset. Perhaps the spots made them too distinctive.



Fig-8 Similar dog breeds (in order of: Malamute, Huskey, Italian Greyhound, and Whippet)

An important fact about the Stanford Dog Breed dataset is that it is a subset of ImageNet-1000, a thousand class dataset of 32,326 images, which itself is a subset of the main ImageNet (14 million images over 20 thousand classes). ImageNet-1000 has become a standard for papers, competitions, and pretrained CNN models in deep learning libraries. Therefore, Keras models already support the 120 Stanford dog classes out of the box. However, they will have the drawback of sometimes predicting one of the 880 non-dog classes. This condition will be studied and remedied with transfer learning.

ImageNetV2 Dog Breed Dataset

Besides the previous data, CIFAR-10 and CIFAR-100 are also both subsets of ImageNet. Since it is so pervasive in industry, there is concern that some results over the years were adaptively overfit to it without knowing. A group out of UC Berkeley developed ImageNetV2 (aka V2), an independent dataset with a matching class structure and published results (Roelofs, 2019):

We evaluate a broad range of models and find accuracy drops of 3% – 15% on CIFAR-10 and 11% – 14% on ImageNet. However, accuracy gains on the original test sets translate to larger gains on the new test sets. Our results suggest that the accuracy drops are not caused by adaptivity, but by the models’ inability to generalize to slightly “harder” images than those found in the original test sets.

This thesis will use the dog breed images in V2, but just as an additional test set because there are only ten images per class. The data seems similar to the Stanford dog data but does seem to have more adversarial examples (Fig-9), and an annoying number of images with two dogs either different species or at least different colors.



Fig-9 V2 Adversarial and Multiple Dog Examples

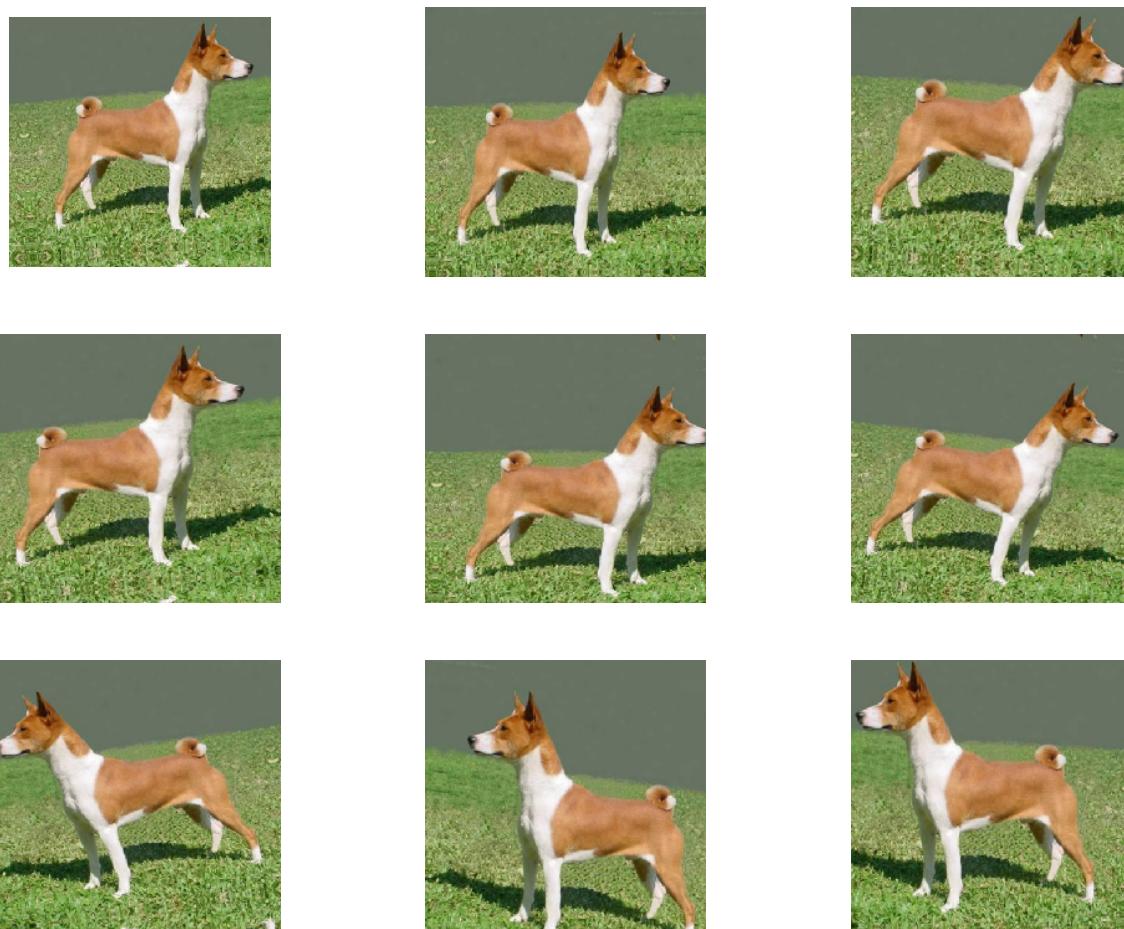
Image Augmentation

The ImageDataGenerator class in the Keras library provides the ability to augment images which hopefully prevents overfit and improves the validation results. Performance will be evaluated on original images and ones augmented with the following settings:

- Horizontal flip = True -- Dogs will sometimes flip between left and right
- Vertical flip = False -- Upside down dogs do not provide value
- Width shift range = 0.1 -- Shift left or right up to 10%
- Height shift range = 0.1 -- Shift up or down up to 10%
- Rotation range = 10.0 -- Rotate up to 10 degrees in either direction
- Shear range = 0.05 – 5 degrees shear angle in counter-clockwise direction
- Zoom range = 0.1 – Random zoom between 90 and 110%
- Fill mode = reflect – Fill points outside input boundaries in an *abcdccba* pattern

The flips, shifts, rotations and zooms are evident in the nine examples below (fig-10).

Figure 10: Augmentation Demo



Basic CNN Image Classification Experiments

To establish a baseline for the pretrained models, a moderate size CNN model was trained from scratch for both original and augmented data. It performs five convolutions on the image all with a 3x3 filter and stride of 1. After each is a max pooling layer with a 2x2 size and stride of 2, which cuts the x and y dimensions in half each time. The last volume is flattened and passed to a batch-normalized dense layer with either 5 or 120 nodes for each possible class. (Fig-11). This is a stripped-down version of the VGG19 architecture which also has five pooling layers but performs multiple convolutions between them.

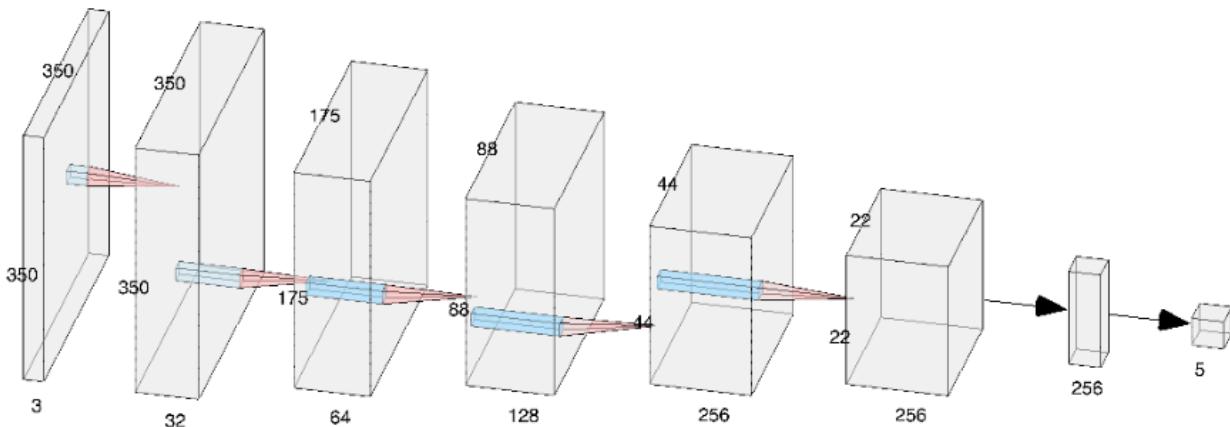


Fig 11: Data flow through basic CNN

Flower Data

The Flower data was trained for 100 epochs with both direct and augmented data. Epoch runs times were about 30 and 90 seconds respectively, so augmentation triples the training time. The learning curves for both are plotted in Fig-12. For training data, the direct case shows an elbow at nearly 0 indicating overfitting while the augmented case gradually decreases due to shifting training data. The validation cost function is very volatile for both, but the direct data shows a net rising trend, another indicator of overfitting which is much smaller in the augmented data

Fig 12a: Basic CNN Learning Curve, no augmentation

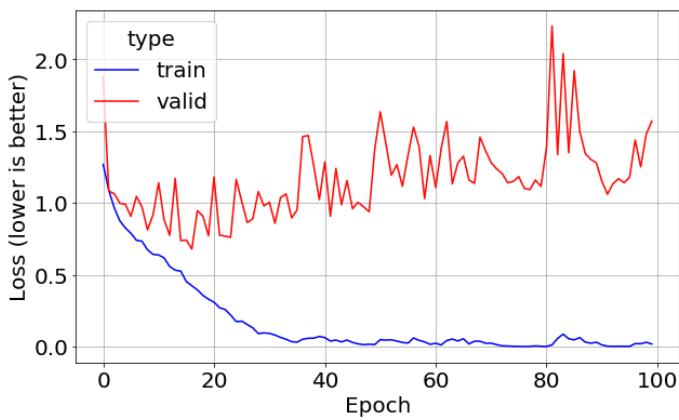
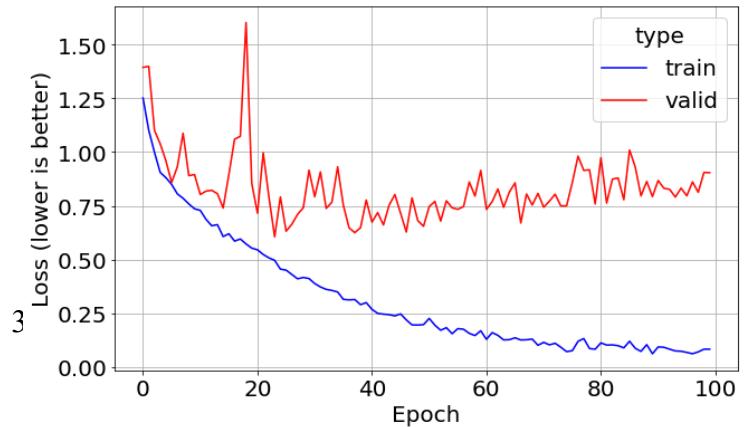


Fig 12b: Basic CNN Learning Curve, augmented



The accuracies of the top and top-2 predictions were collected. Augmented validation (fig-14) was about 79% which was higher and more steady than direct at approximately 74%. The training result for direct shows a knee corresponding to the elbow in the learning curve. Top-2 results show the same trends as the top ones.

The fact that the training data converges to 1 or nearly 1 is evidence that this five-convolution design is powerful enough to memorize the 3026 training samples. If more powerful architectures were not available, the next task would be seeing if stronger regulation moved the train and validation results closer together.

A second dense layer of 256 nodes was added, but performance stayed the same, just under 80% validation accuracy.

Fig 13: Basic CNN Model Accuracy, no augmentation

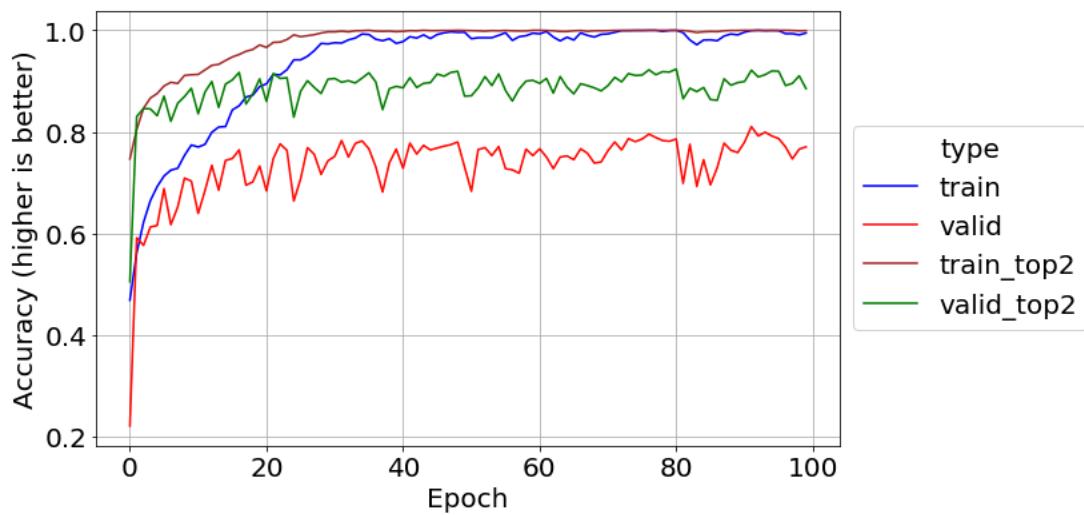
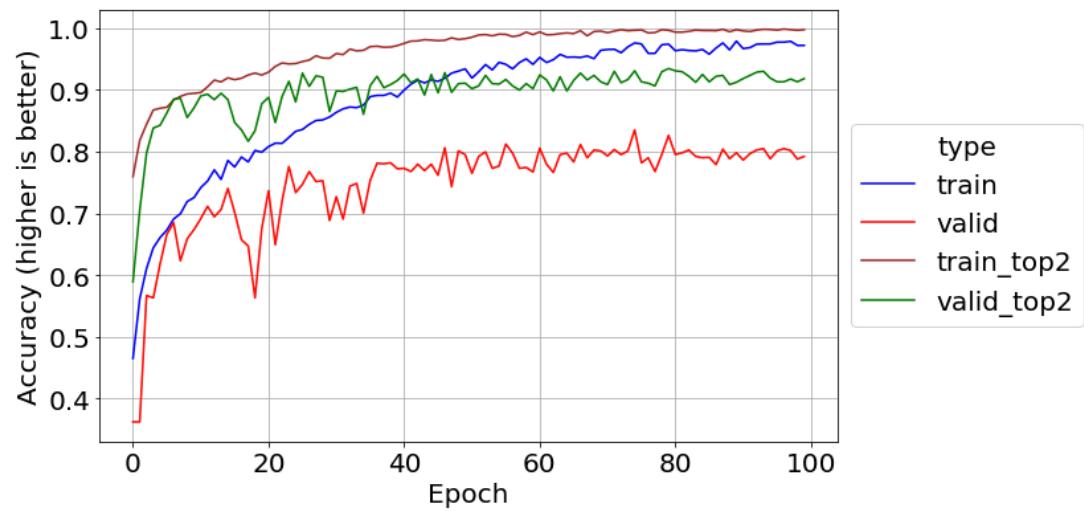


Fig 14: Basic CNN Model Accuracy, augmented



Stanford Dog Breed Data

The previous activities were repeated for the Stanford data which is much larger, but has 115 more classes and less samples per class, about 180 vs about 600.

Fig 15a: Basic CNN Learning Curve, (dog, direct)

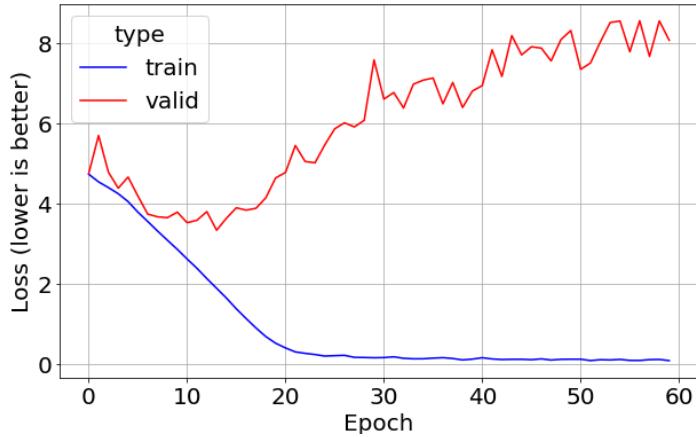


Fig 15b: Basic CNN Learning Curve, (dog, augment)

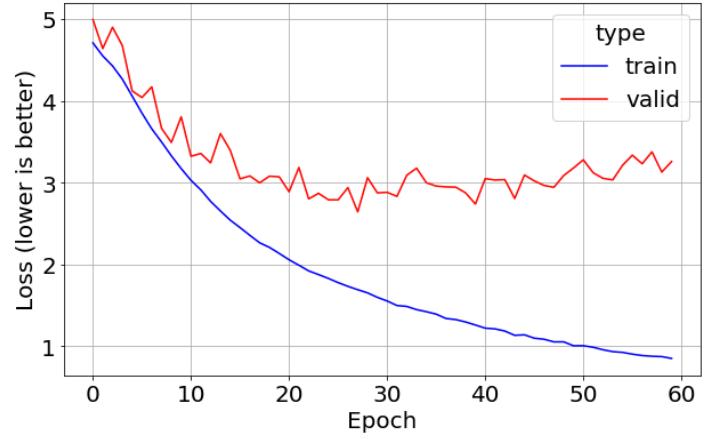


Fig 16: Basic CNN Model Accuracy, (dog, direct)

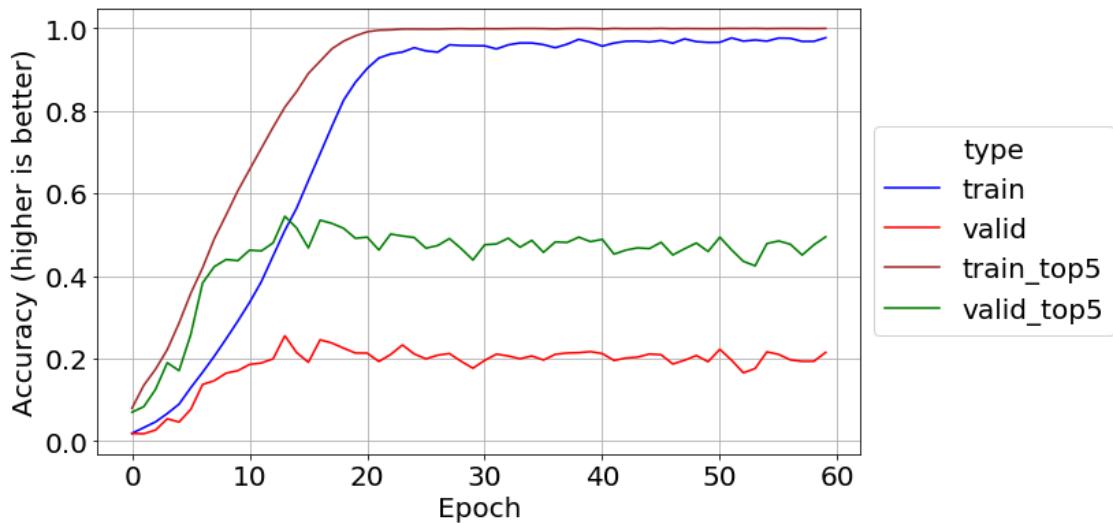
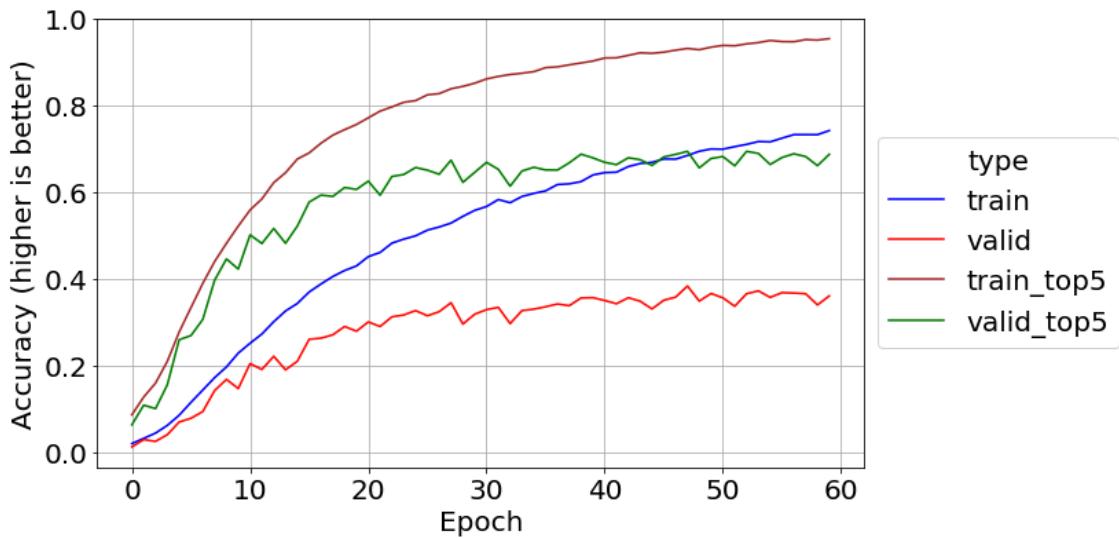
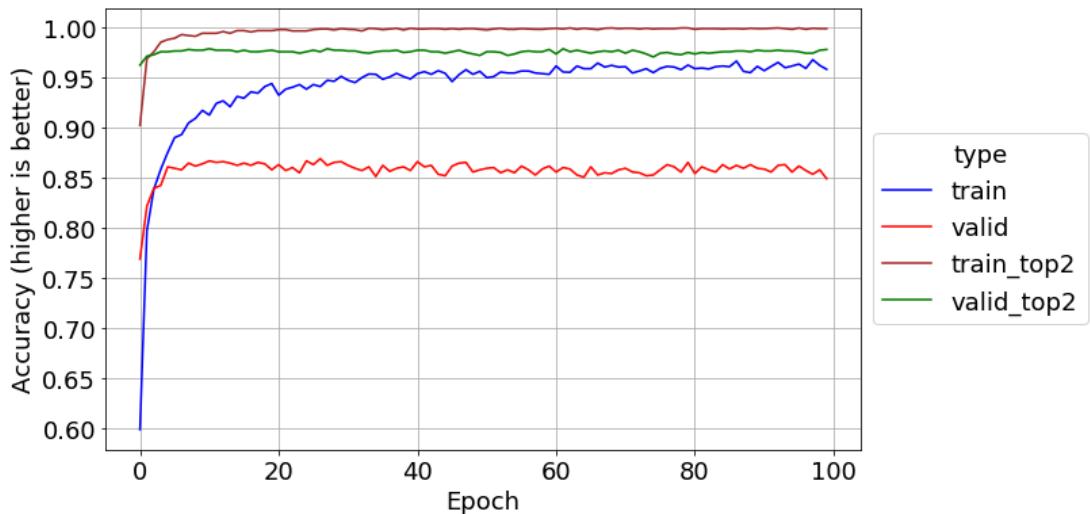


Fig 17: Basic CNN Model Accuracy, (dog, augment)



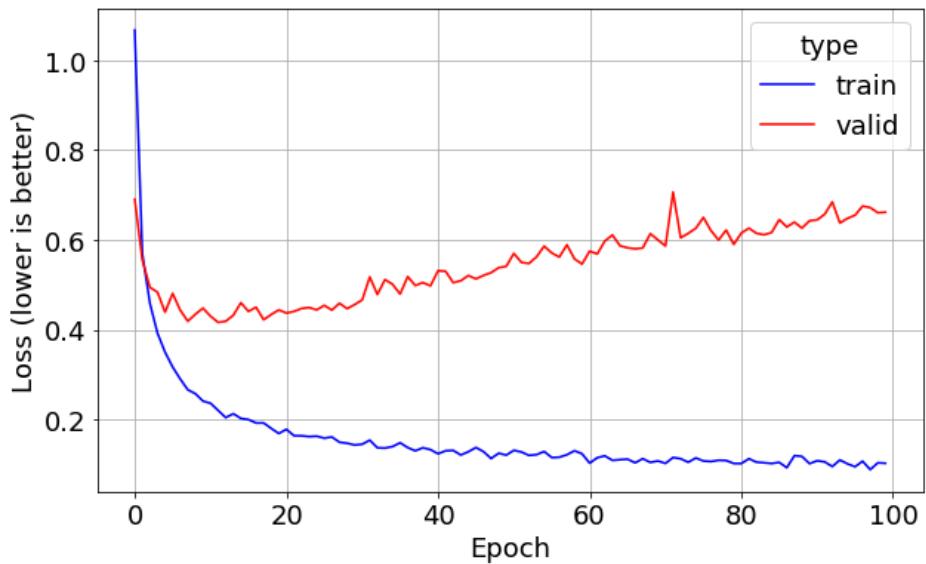
<https://neurohive.io/en/popular-networks/vgg16/>

Model Accuracy

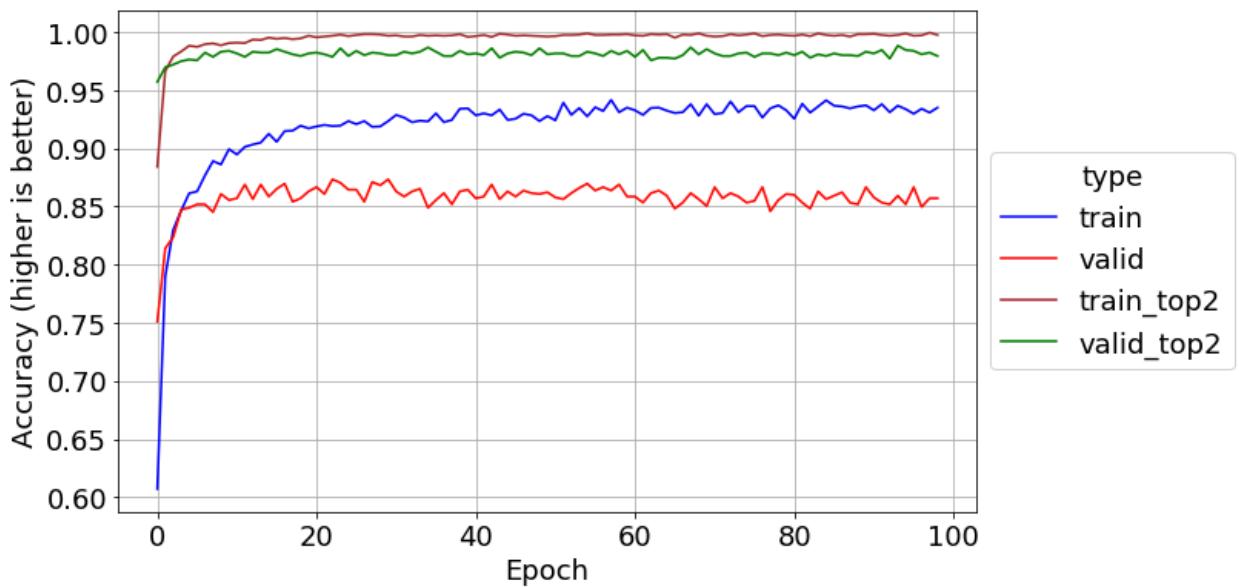


Flower vgg19

Learning Curve

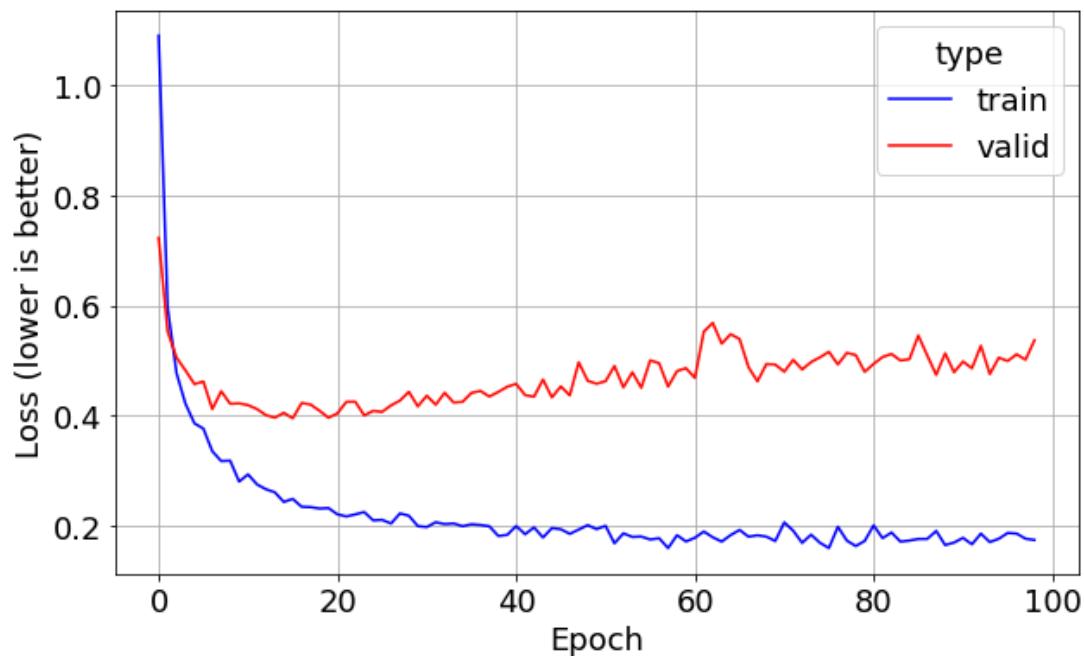


Model Accuracy

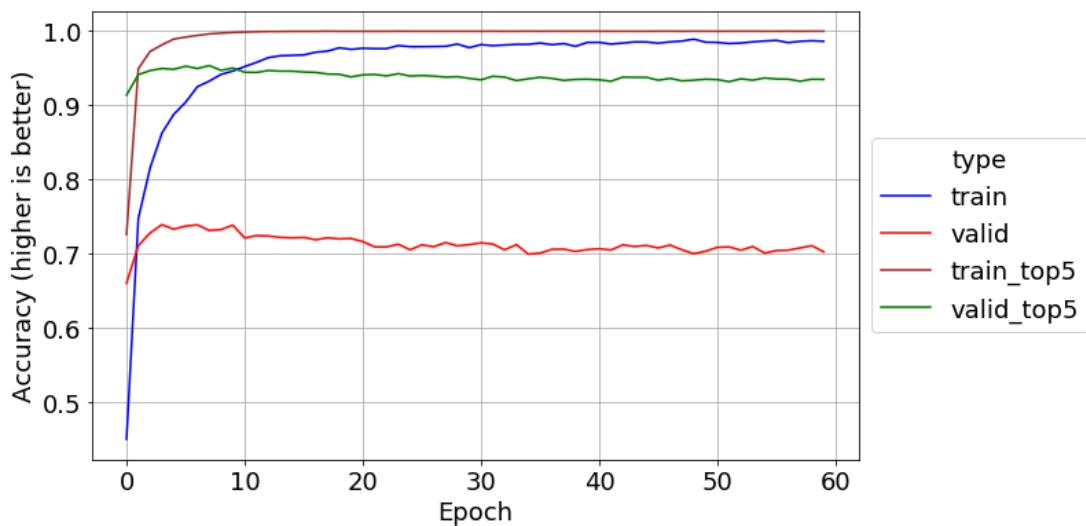


Flower da vgg19

Learning Curve

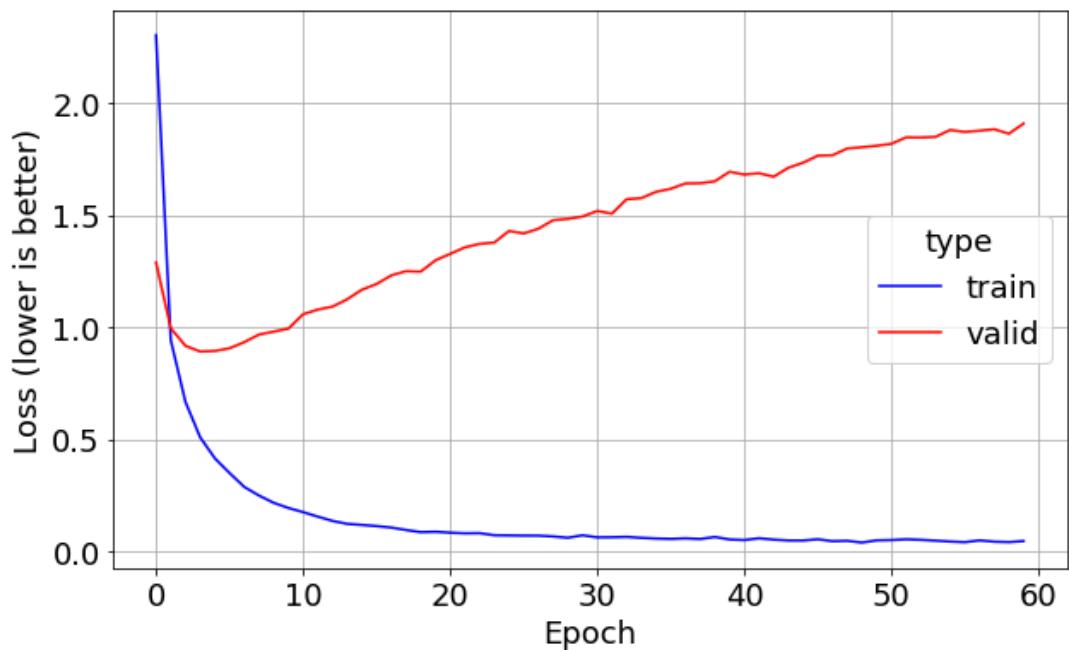


Model Accuracy

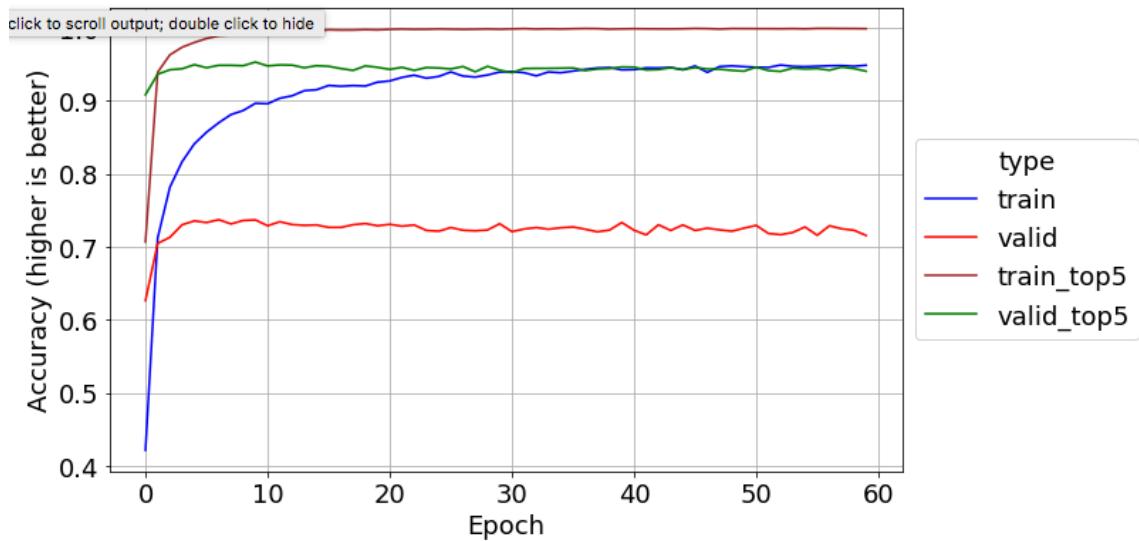


Stanford vgg19

Learning Curve

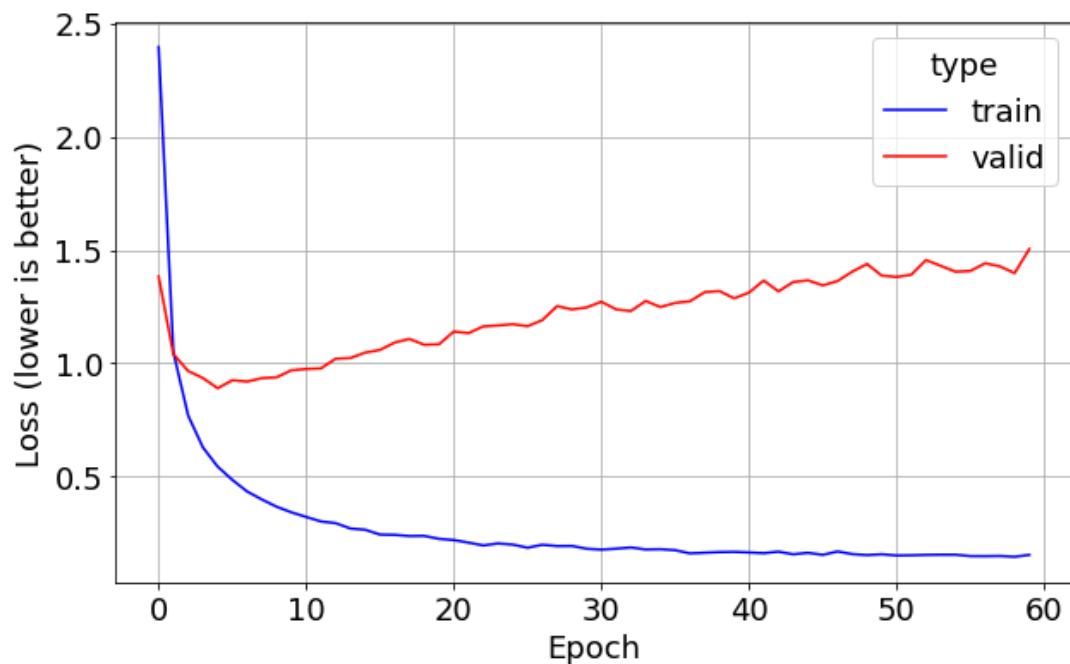


Model Accuracy

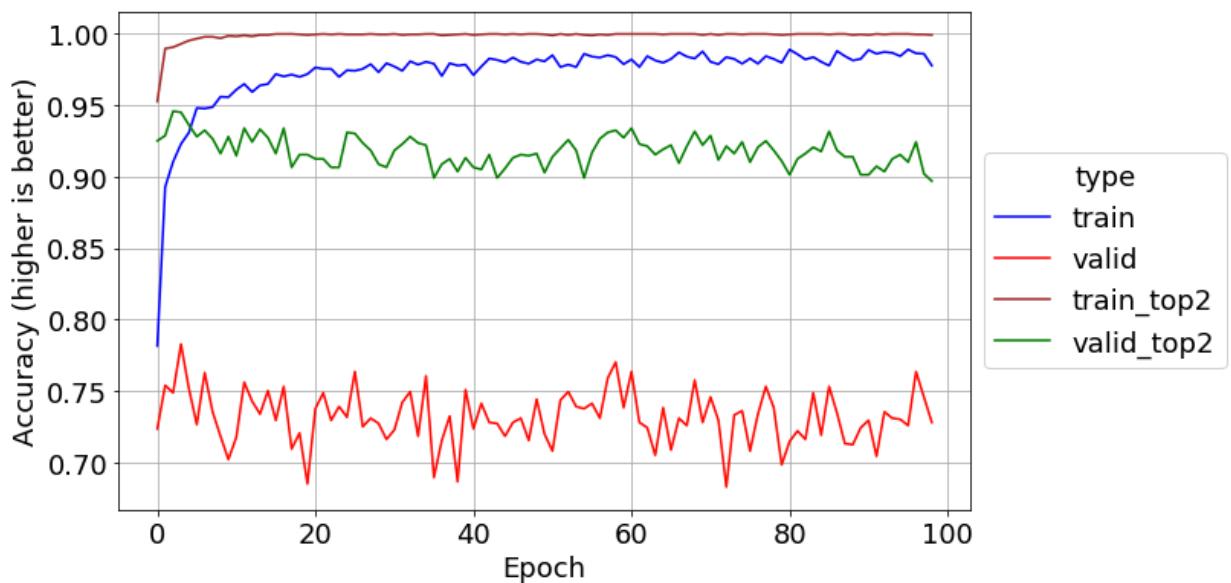


Stanford da vgg19

Learning Curve

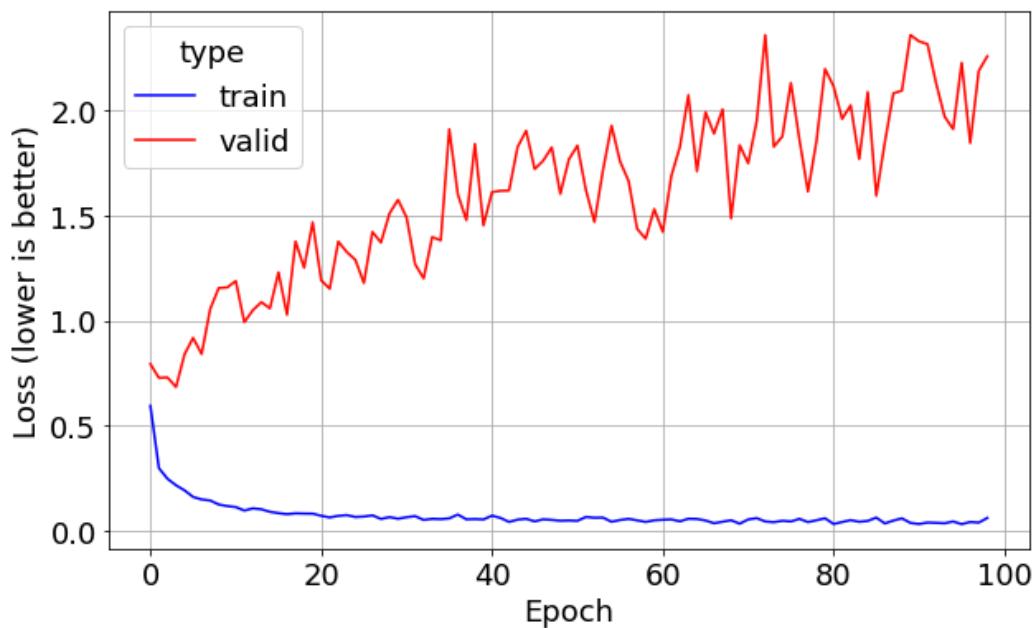


Model Accuracy

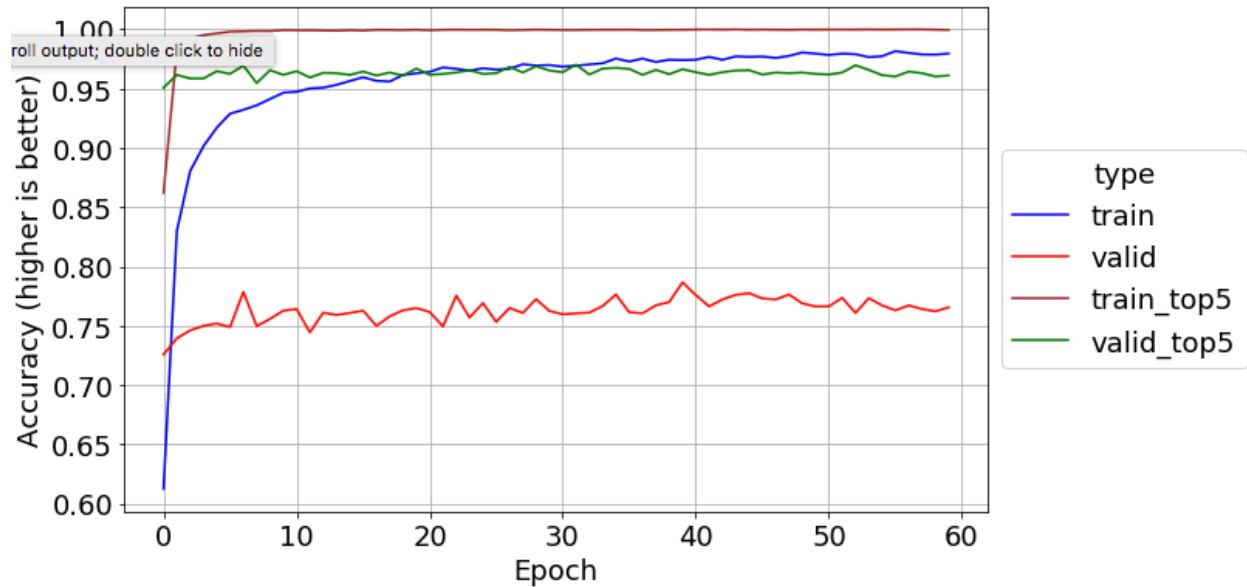


Flower_da_resnet

Learning Curve

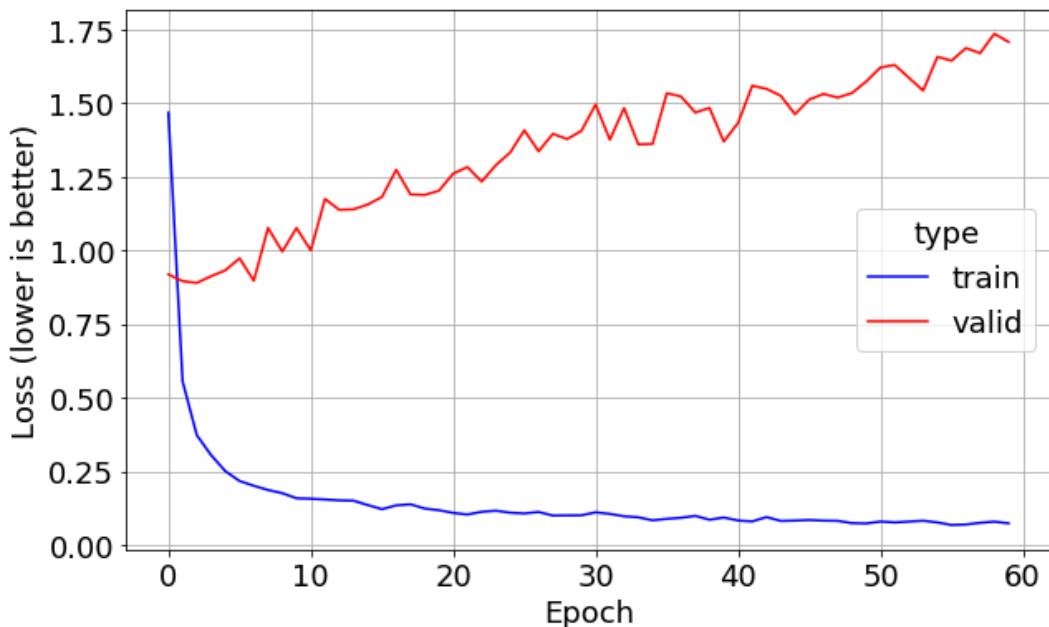


Model Accuracy

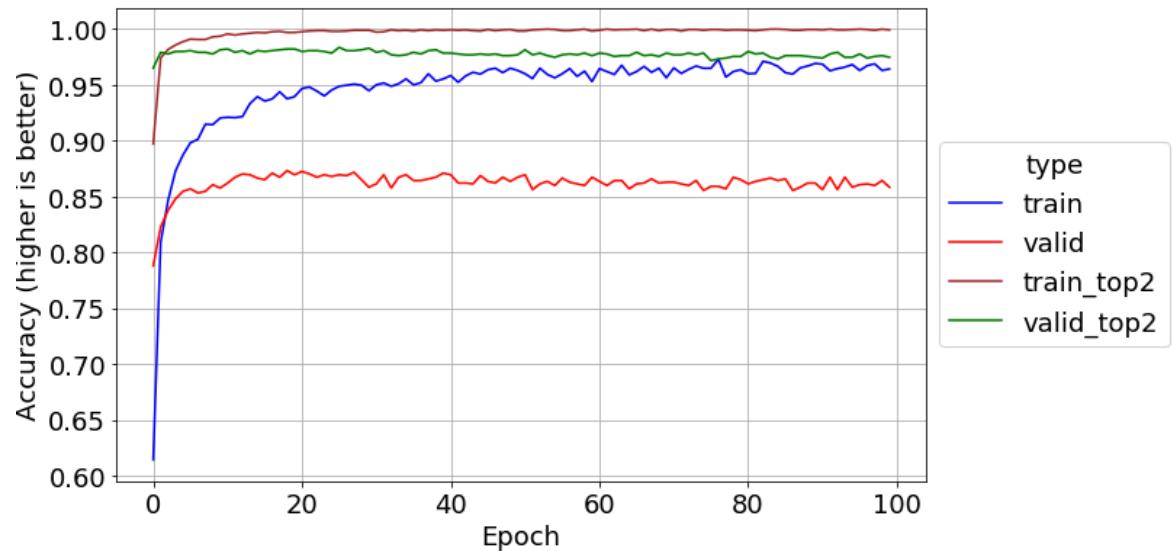


Stanford da Resnet50

Learning Curve

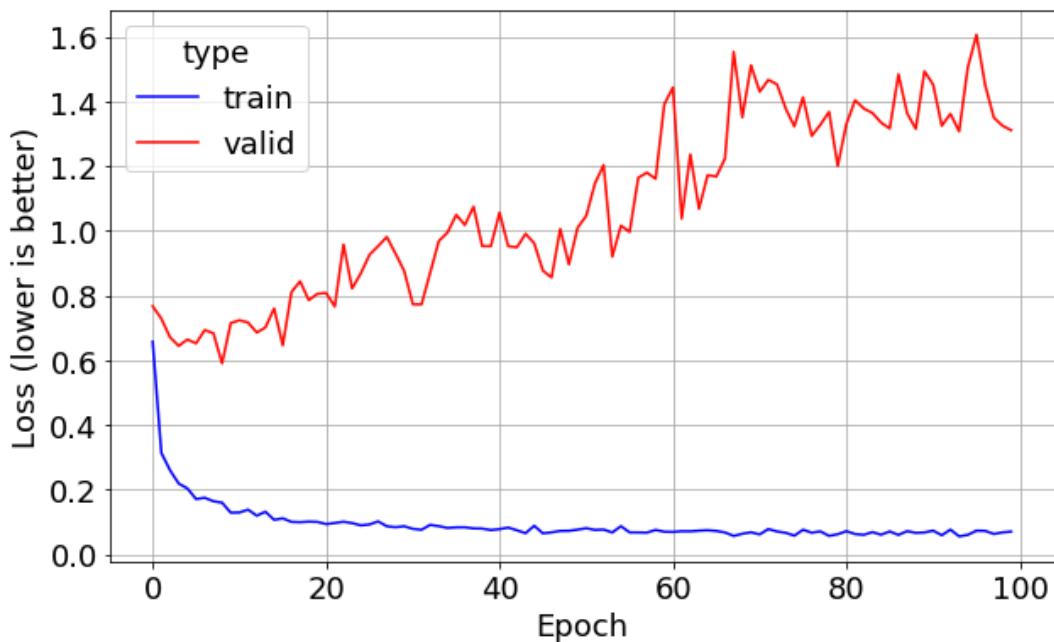


Model Accuracy

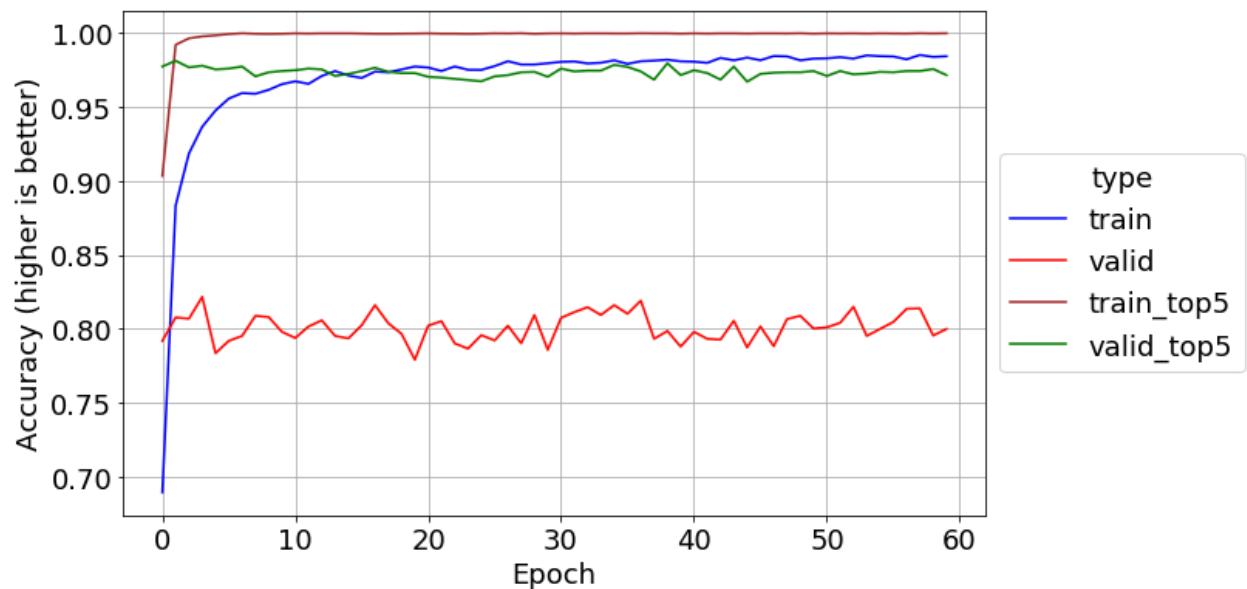


Flowers DA Densenet201

Learning Curve

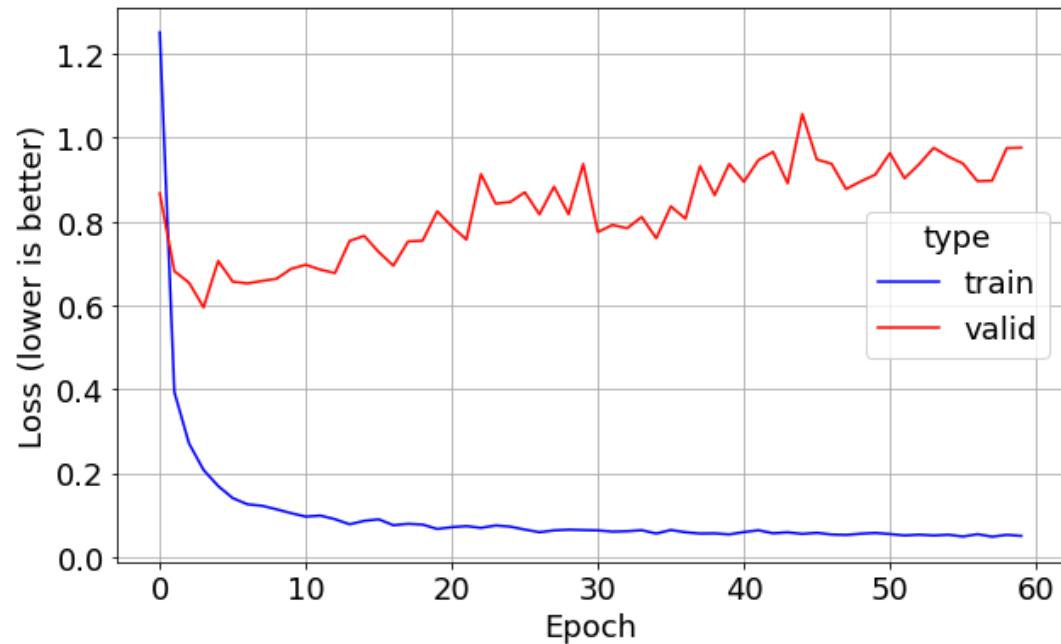


Model Accuracy

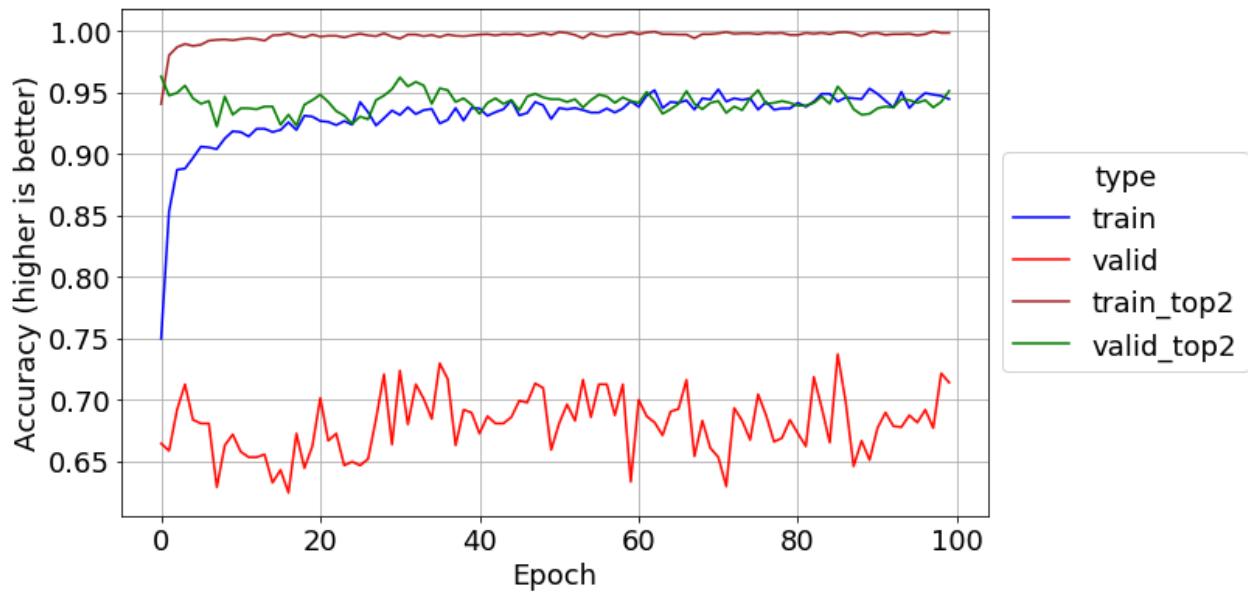


Stanford da DenseNet201

Learning Curve

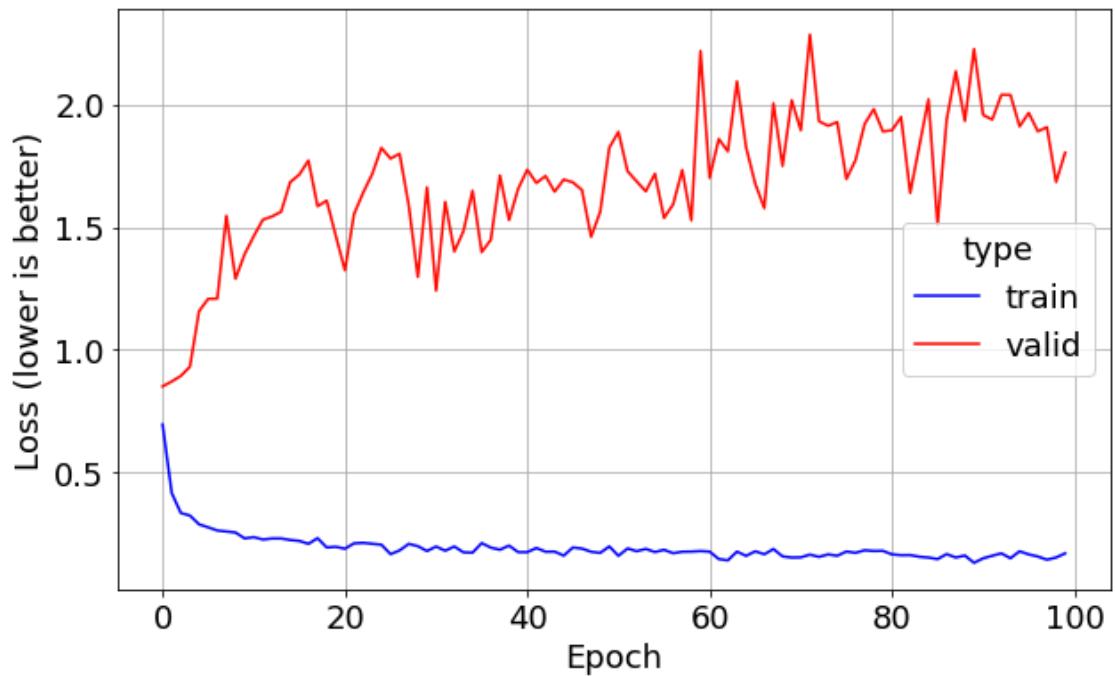


Model Accuracy



Flowers da inceptionV3

Learning Curve



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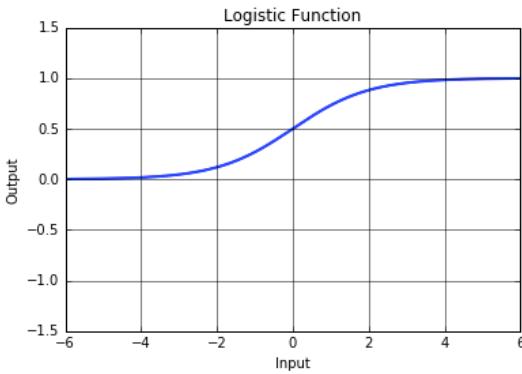
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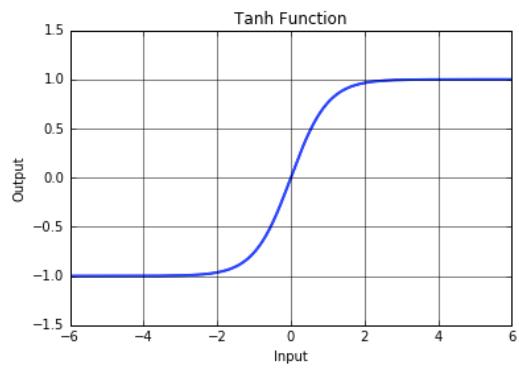
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Appendix



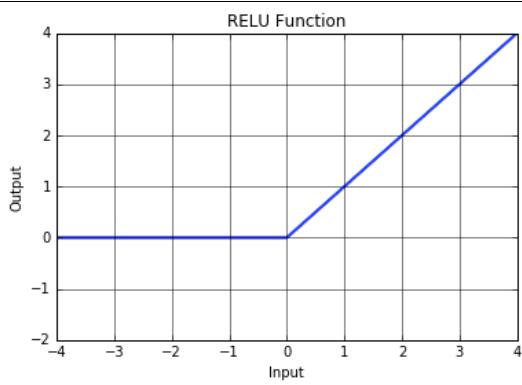
$$Y = \frac{1}{1 + e^{-x}}$$

$$Y' = Y * (1 - Y)$$



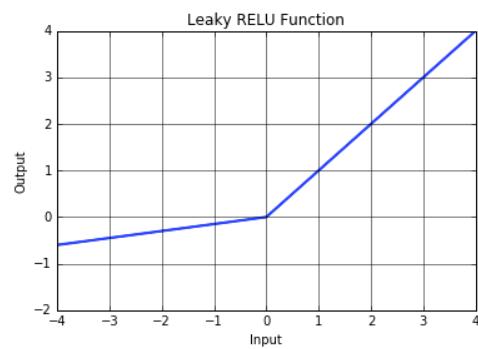
$$Y = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

$$Y' = 1 - Y^2$$



$$Y = x * (x > 0)$$

$$Y' = 1 * (x > 0)$$



$$Y = x * (0.15 * (x < 0) + (x > 0))$$

$$Y' = 0.15 * (x < 0) + 1 * (x > 0)$$

```

# Define input and output data for XOR function
x = np.array([[0, 0], [0, 1], [1, 0], [1, 1]])
y = np.array([[0], [1], [1], [0]])

input_layer_size = 2
hidden_layer_size = 4
output_layer_size = 1

# Randomly initialize 2-D weight matrices
np.random.seed(2)
h_weights = np.random.randn(input_layer_size, hidden_layer_size)
y_weights = np.random.randn(hidden_layer_size, output_layer_size)

for t in range(2001):
    # Predict Y with forward propagation
    h_linear = x.dot(h_weights)           # weighted sum of two inputs
    h_relu = np.maximum(h_linear, 0)       # ReLU activation function
    y_linear = h_relu.dot(y_weights)       # weighted sum of 4 hidden layer neurons
    y_pred = y_linear                     # no activation function, passing thru

    # Compute and print loss
    loss = 0.5 * np.square(y - y_pred).sum()
    relu.pretty_print(t, loss, y_pred)

    # Back-propagate to find gradients of h and y weights wrt loss
    y_delta = (y_pred - y) * 1.0          # loss derivative * pass-thru derivative
    y_weight_gradient = h_relu.T.dot(y_delta)

    h_delta = y_delta.dot(y_weights.T) * 1.0 # ReLU derivative is either 1 or 0
    h_delta[h_linear < 0] = 0
    h_weight_gradient = x.T.dot(h_delta)

    # Update weights with product of learning rate and gradient
    h_weights -= 0.002 * h_weight_gradient
    y_weights -= 0.002 * y_weight_gradient

```

Dataset Links

Flowers

<https://www.kaggle.com/alxmamaev/flowers-recognition>

Stanford Dog Breeds

<http://vision.stanford.edu/aditya86/ImageNetDogs>

ImageNet V2

<https://github.com/modestyachts/ImageNetV2>

Full list of ImageNet 1000 classes (for informational purpose)

<https://gist.github.com/yrevar/942d3a0ac09ec9e5eb3a>

breed_1	n_samples_1	breed_2	n_samples_2	breed_3	n_samples_3
affenpinscher	150	bouvier_des_flandres	150	english_setter	161
afghan_hound	239	boxer	151	english_springer	159
african_hunting_dog	169	brabancon_griffon	153	entlebucher	202
airedale	202	briard	152	eskimo_dog	150
american_staffordshire_terrier	164	brittany_spaniel	152	flat-coated_retriever	152
appenzeller	151	bull_mastiff	156	french_bulldog	159
australian_terrier	196	cairn	197	german_shepherd	152
basenji	209	cardigan	155	german_short-haired_pointer	152
basset	175	chesapeake_bay_retriever	167	giant_schnauzer	157
beagle	195	chihuahua	152	golden_retriever	150
bedlington_terrier	182	chow	196	gordon_setter	153
bernese_mountain_dog	218	clumber	150	great_dane	156
black-and-tan_coonhound	159	cocker_spaniel	159	great_pyrenees	213
blenheim_spaniel	188	collie	153	greater_swiss_mountain_dog	168
bloodhound	187	curly-coated_retriever	151	groenendael	150
bluetick	171	dandie_dinmont	180	ibican_hound	188
border_collie	150	dhole	150	irish_setter	155
border_terrier	172	dingo	156	irish_terrier	169
borzoi	151	doberman	150	irish_water_spaniel	150
boston_bull	182	english_foxhound	157	irish_wolfhound	218

breed_1	n_samples_1	breed_2	n_samples_2	breed_3	n_samples_3
italian_greyhound	182	norwegian_elkhound	196	shih-tzu	214
japanese_spaniel	185	norwich_terrier	185	siberian_husky	192
keeshond	158	old_english_sheepdog	169	silky_terrier	183
kelpie	153	otterhound	151	soft-coated_wheaten_terrier	156
kerry_blue_terrier	179	papillon	196	staffordshire_bullterrier	155
komondor	154	pekingese	149	standard_poodle	159
kuvasz	150	pembroke	181	standard_schnauzer	155
labrador_retriever	171	pomeranian	219	sussex_spaniel	151
lakeland_terrier	197	pug	200	tibetan_mastiff	152
leonberg	210	redbone	148	tibetan_terrier	206
lhasa	186	rhodesian_ridgeback	172	toy_poodle	151
malamute	178	rottweiler	152	toy_terrier	172
malinois	150	saint_bernard	170	vizsla	154
maltese_dog	252	saluki	200	walker_hound	153
mexican_hairless	155	samoyed	218	weimaraner	160
miniature_pinscher	184	schipperke	154	welsh_springer_spaniel	150
miniature_poodle	155	scotch_terrier	158	west_highland_white_terrier	169
miniature_schnauzer	154	scottish_deerhound	232	whippet	187
newfoundland	195	sealyham_terrier	202	wire-haired_fox_terrier	157
norfolk_terrier	172	shetland_sheepdog	157	yorkshire_terrier	164

