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
Tbd2

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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 at 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 log2(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. It's 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:

$$F(x_1 + cx_2) = F(x_1) + cF(x_2) \tag{1}$$

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 equation:

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

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.

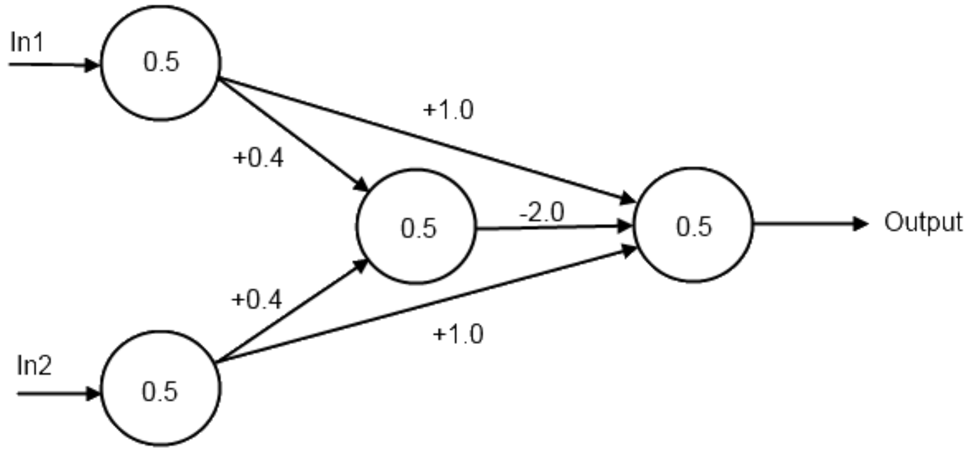


Fig 1: Hidden Layer Providing Exclusive-OR Operation

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

The creation of a functional neural network involves two interleaved steps, each using a dedicated labeled subset of the full data. Each is run through the model (forward propagation) to produce outputs which can be compared to the ground-truth labels. The first step uses training data to determine the correct node weights and biases. 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 validation results. 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 nearly the same 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).

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 output a 0 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 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 reason is that backpropagation computes the cost function with respect to all weights and biases through repeated application of 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:

$$\frac{dz}{dx} = \frac{dz}{dy} * \frac{dy}{dx} \tag{3}$$

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):

$$\mathrm{z} - \text{weighted sums at a layer}$$
$$\sigma - \text{nonlinear activation function}$$
$$a - \text{output activations for a layer}$$
$$\delta - \text{error vector at point Z}$$
$$\odot - \text{Hadamard (elementwise matrix) product}$$

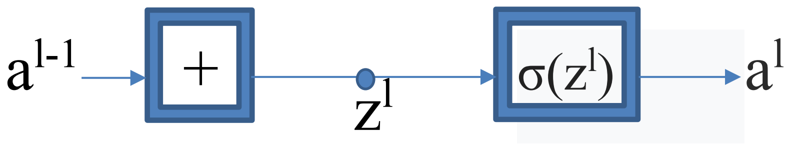


Figure 2: Basic Node Operation

Basic Feedforward NN Equations (for comparison)

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

$$Z^l = w^l a^{l-1} + b^l \tag{4}$$
$$a^l = \sigma(z^l) \tag{5}$$

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 with the activation function's derivative effectively "steps back" the error to point Z^L in the output layer.

$$\delta^L = \nabla_a C \odot \sigma'(z^L) \tag{6}$$

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.

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

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.

$$\frac{\partial C}{\partial b} = \delta \tag{8}$$

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

The last equation finally 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 the current weight value is shifted by. As the cost function approaches a minimum (local or global), its derivative becomes smaller due to a smaller error term and produces a smaller 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.

$$\frac{\partial C}{\partial w} = a_{in} \delta_{out} \tag{9}$$

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 difference between the predicted and ground truth values works well. Since this point is reached through a single backpropagation operation, the delta is determined by the 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 and a simple quadratic cost function suffices:

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

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:

$$C(clf_{multinomial}) = -\sum Ylog(\hat{Y}) \tag{11a}$$

$$C(clf_{binary}) = -ylog(\hat{y}) - (1 - y)\log(1 - \hat{y}) \tag{11b}$$

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 also 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 the cost function. They claim the better calculations 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, which 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 because this 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 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 less common normalizations available. Batch normalization has become very popular similar to dropout, and is sometimes preferred over it. The dropout amount 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. This 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. 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 is 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.

$$Var(primitive) = 0.1 \tag{12a}$$

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

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

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

Basic Update Equations

Tying together the above information, the basic update formulae for weight and bias are:

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

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

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)

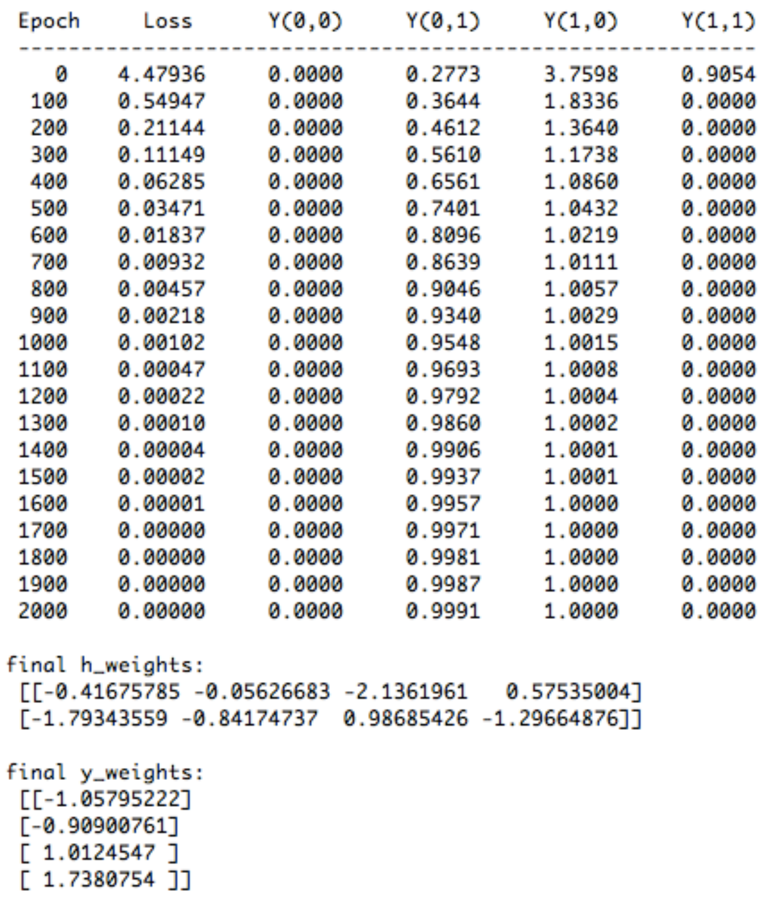
k = fudge factor because some libraries update bias differently than weights

Debugging Tip

When designing a neural network classifier, it helps to verify basic operation with a tiny data subset such as 32 samples (reduced to two classes if multiclass). This 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.

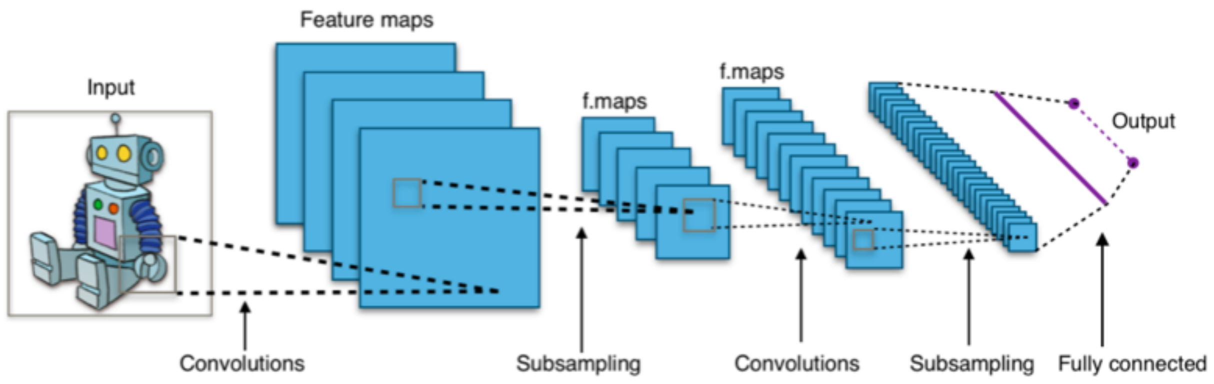


Fig-4: Basic CNN Structure (by Aphex34 - Own work, CC BY-SA 4.0), **https://commons.wikimedia.org/w/index.php?curid=45679374**

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:

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

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 often 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.

1	1	1
1	1	1
1	1	1

(a)

0	-1	0
-1	10	-1
0	-1	0

(b)

0	1	0
1	-4	1
0	1	0

(c)

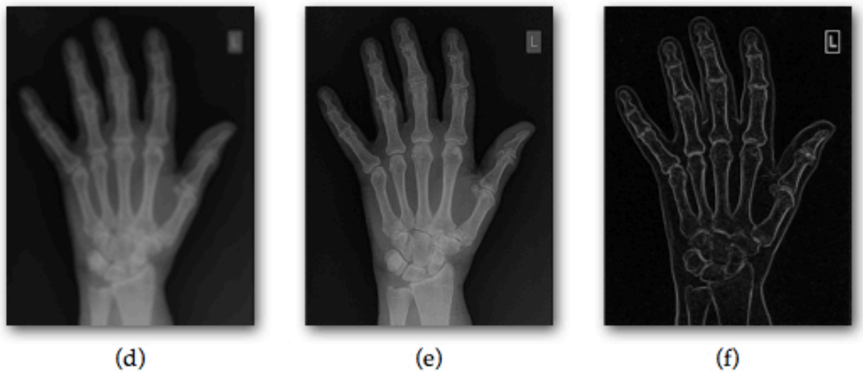


Fig-5: Edge Detection Filters (By Kieranmaher - Own work, Public Domain)
https://commons.wikimedia.org/w/index.php?curid=13305900

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 performed 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.

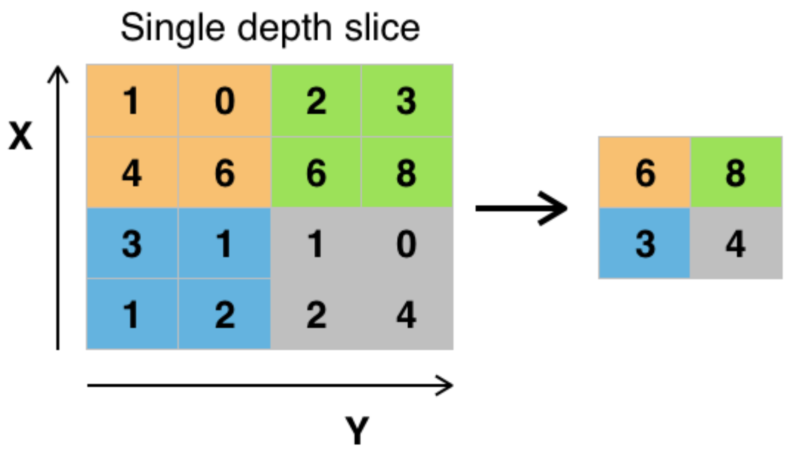


Fig-6: Simple Max-Pooling Example (By Aphex34 - Own work, CC BY-SA 4.0) https://commons.wikimedia.org/w/index.php?curid=45673581

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, one for each possible convolution position, and each one of those connects to one position in the next feature map. Filters in the same stack share weights, while a different feature map will have its own filter stack with the same dimensions but different weights.

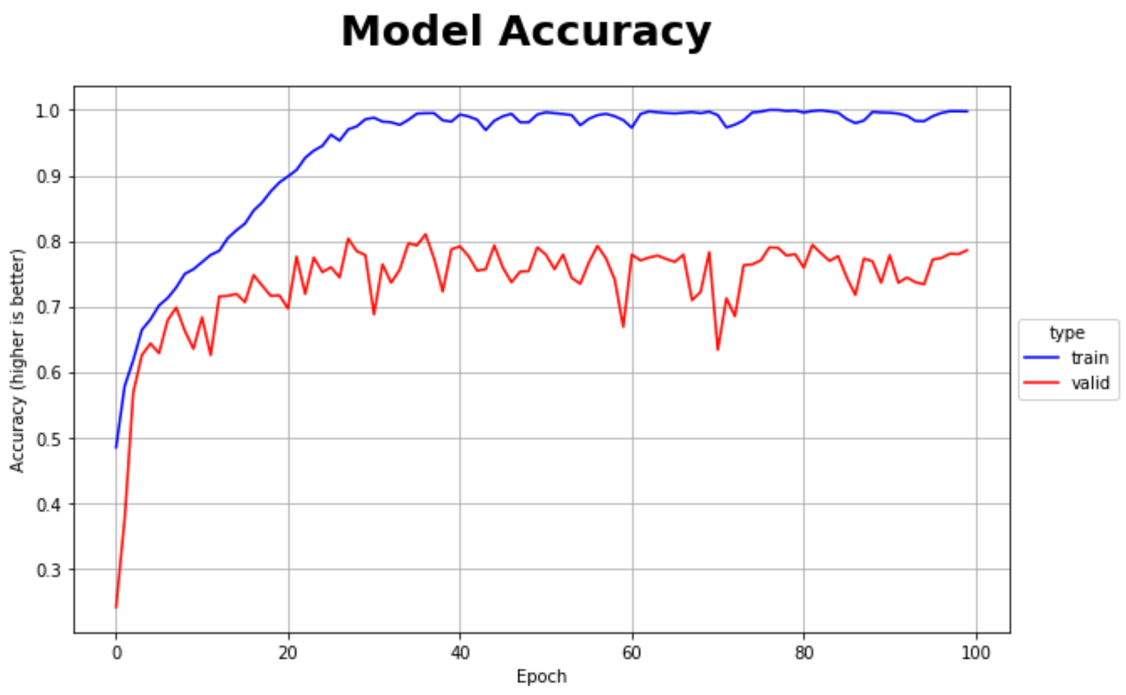
Backpropagation is performed by rotating the filter 180 degrees and performing convolution from back to front. Filters and fully connected nodes are trained while pools and ReLU (if used) are constant.

An example of calculations for one layer is taken from the 2012 ImageNet Challenge winner (Krizhevsky, 2012):

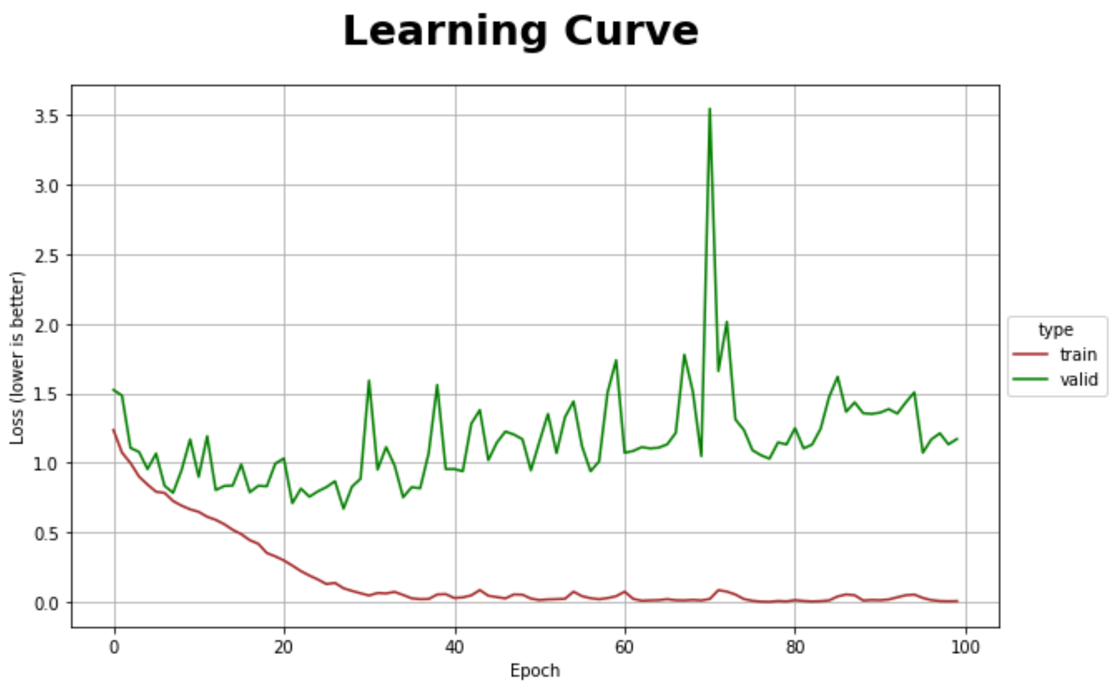
- Image size = 224 * 224 * 3 layers
- Filter size 11 x 11 with stride 4 and double-sided padding of 3
- Output dimension = (224 -11 + 3) / 4 + 1 = 55
- K = 96 feature maps
- Output volume = 55 x 55 x 96
- Unique weights = 11 x 11 x 3 x 96 = 34848
- Unique biases = 96

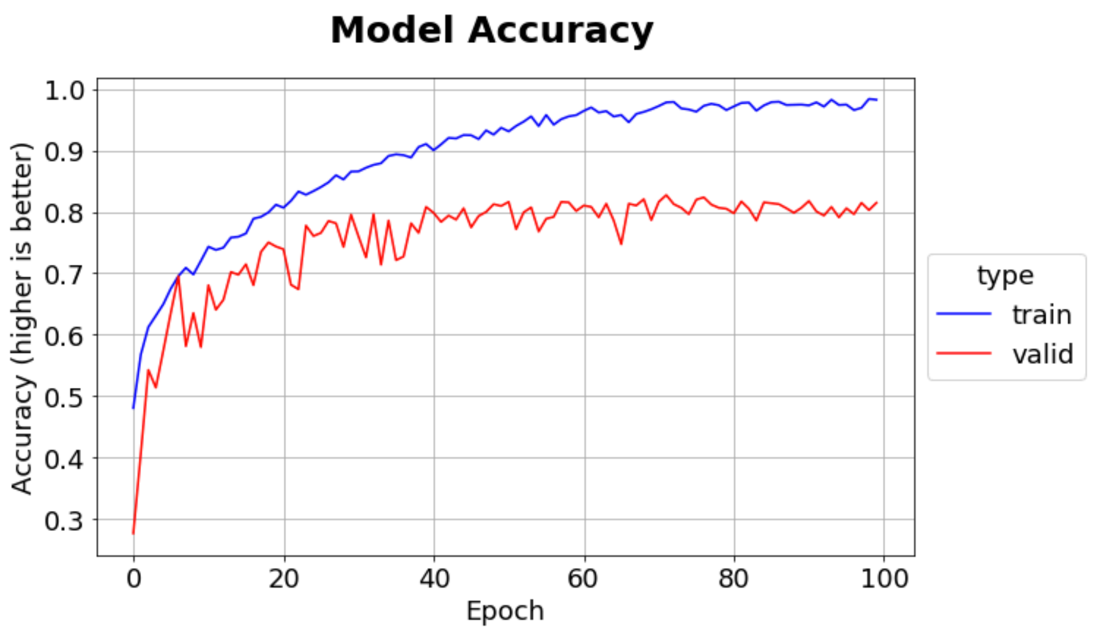
Description of Datasets

Flowers: (70/30)
3026 training over 5 groups
Daisy 539, Dandelion 737, Rose 550, sunflower 515, tulip 690
1329 validation

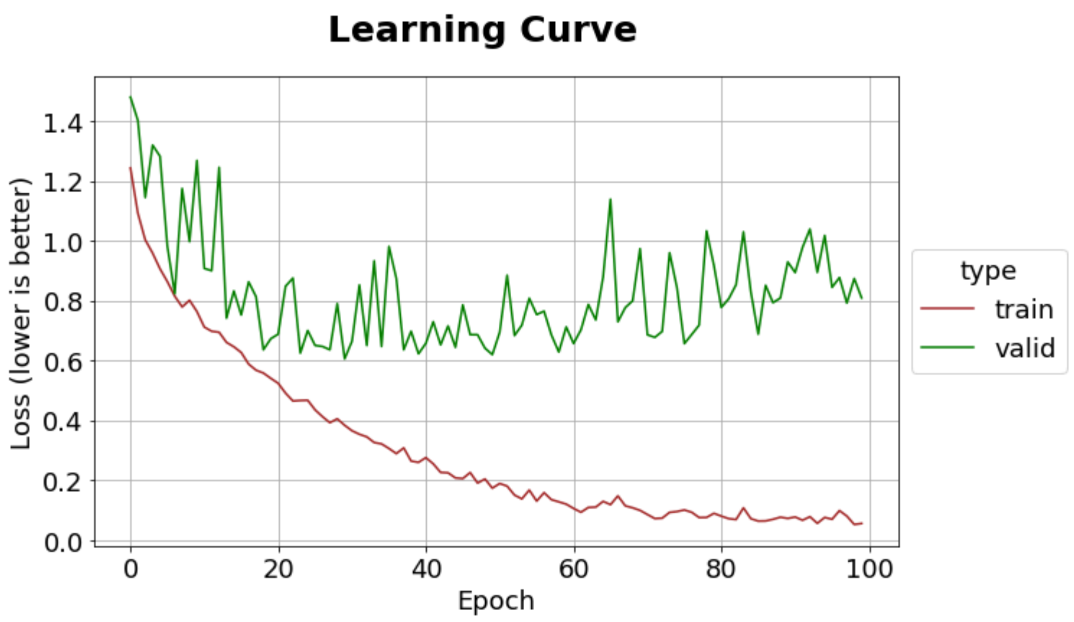


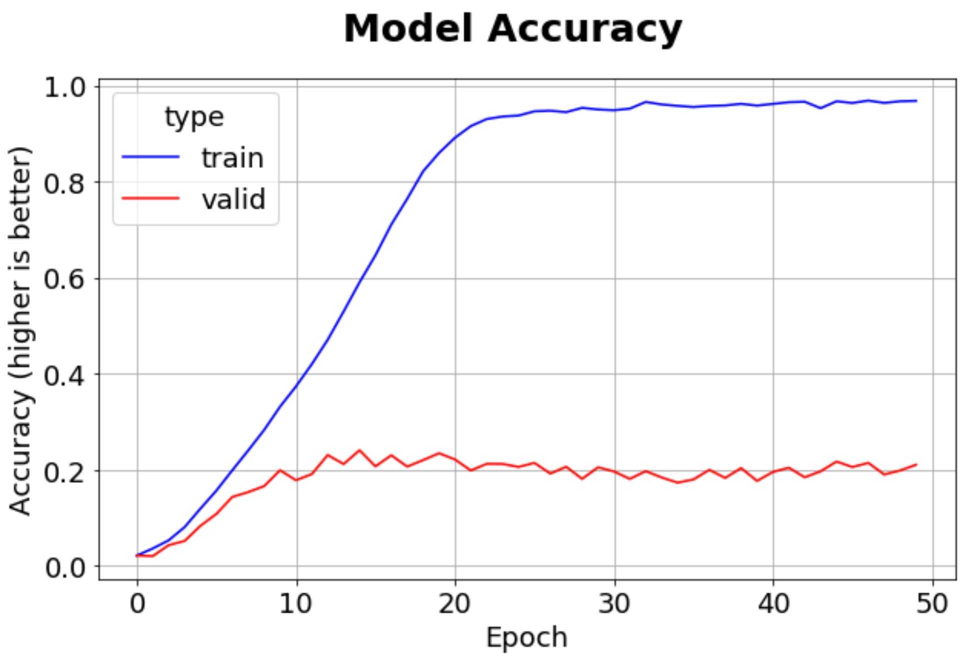
Scratch Flower



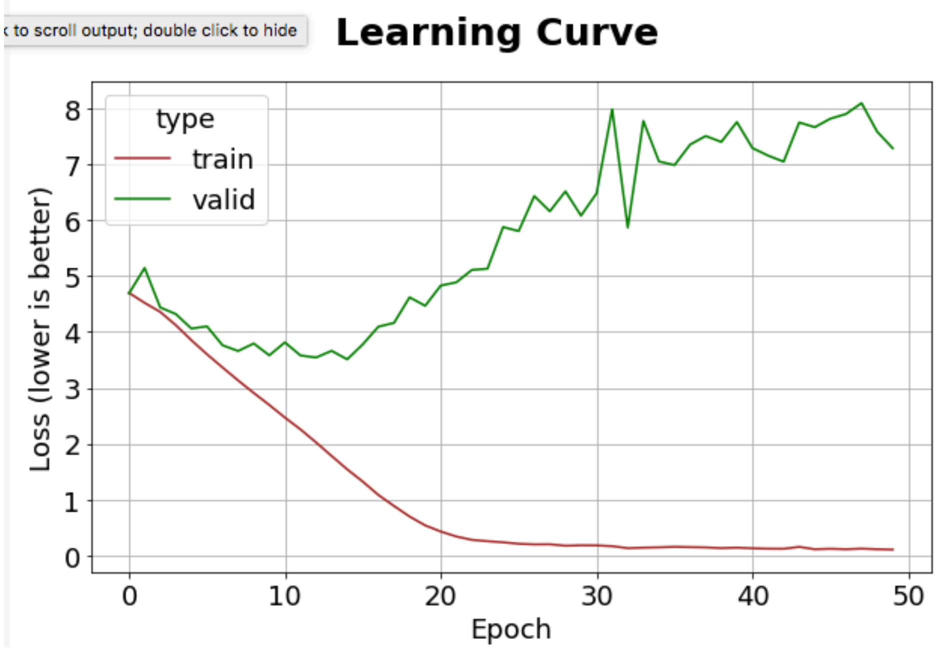


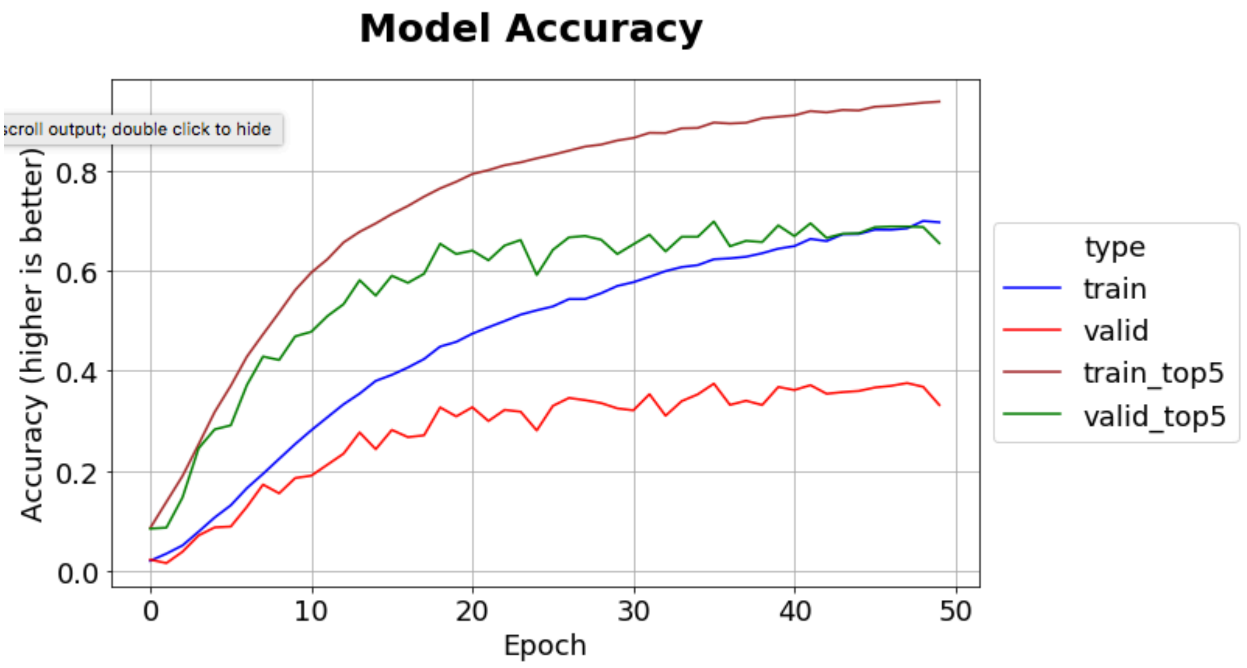
Scratch flower da



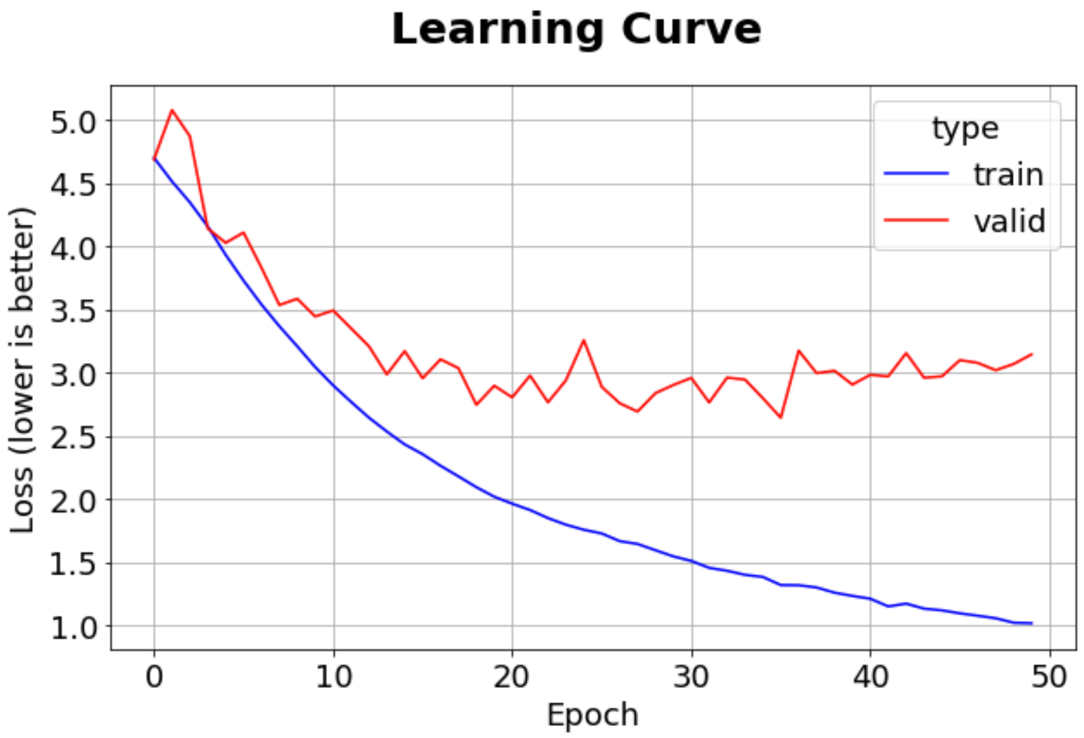


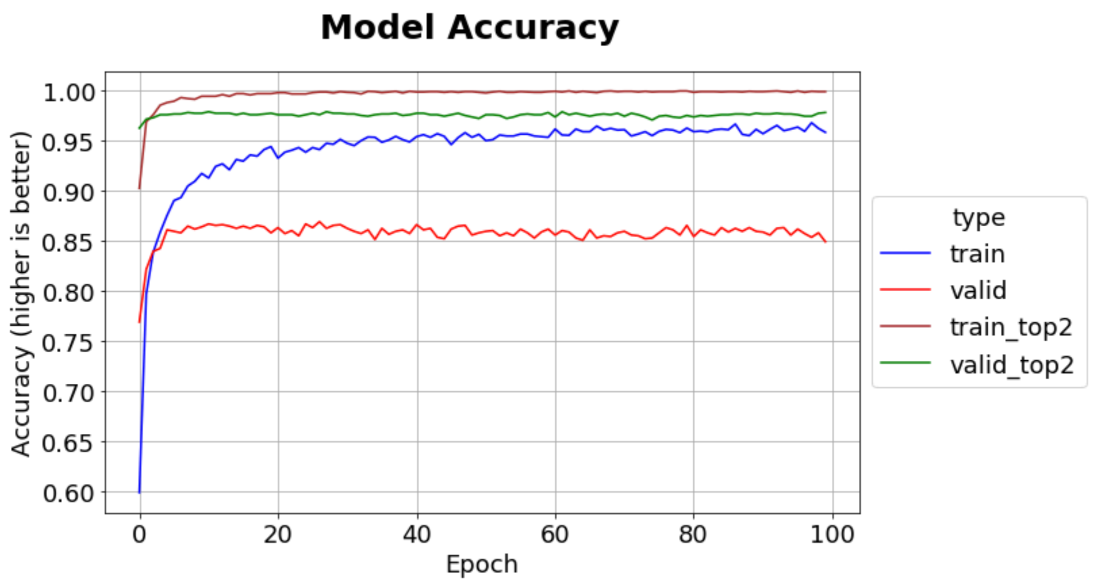
Scratch tanford



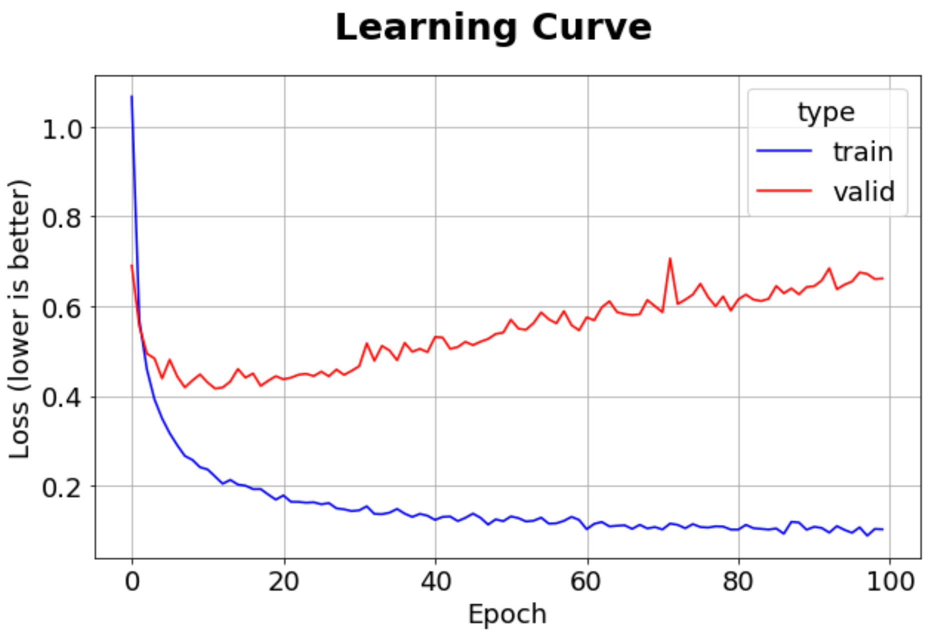


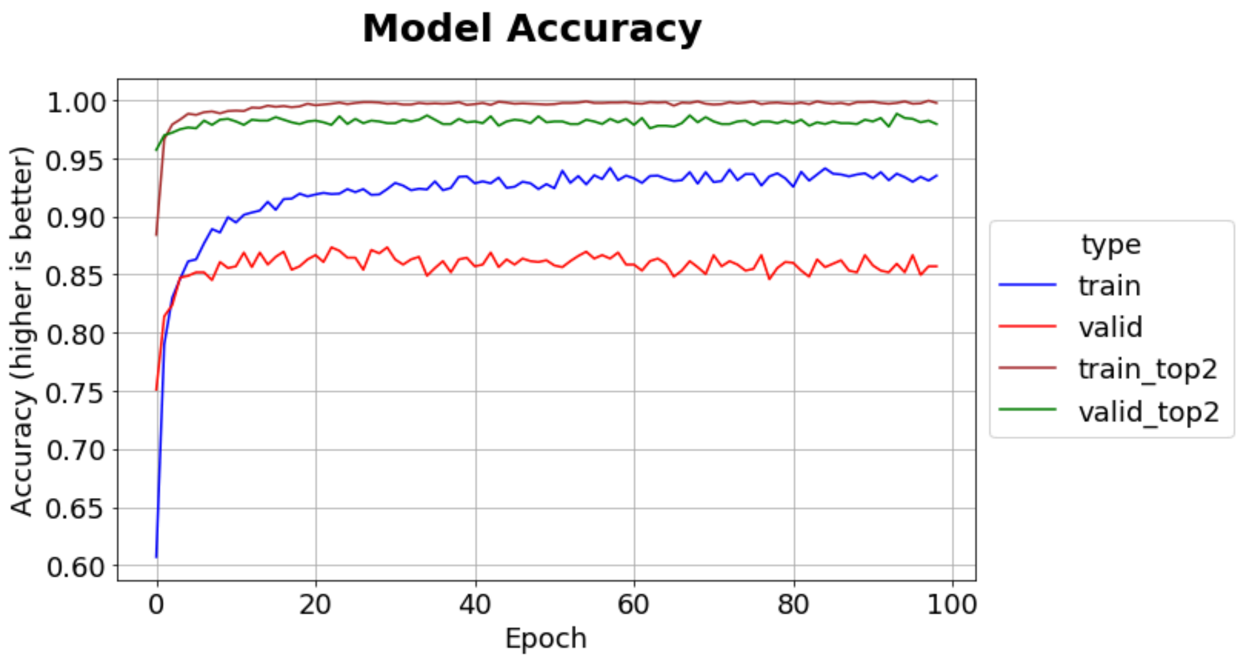
Scratch Stanford da



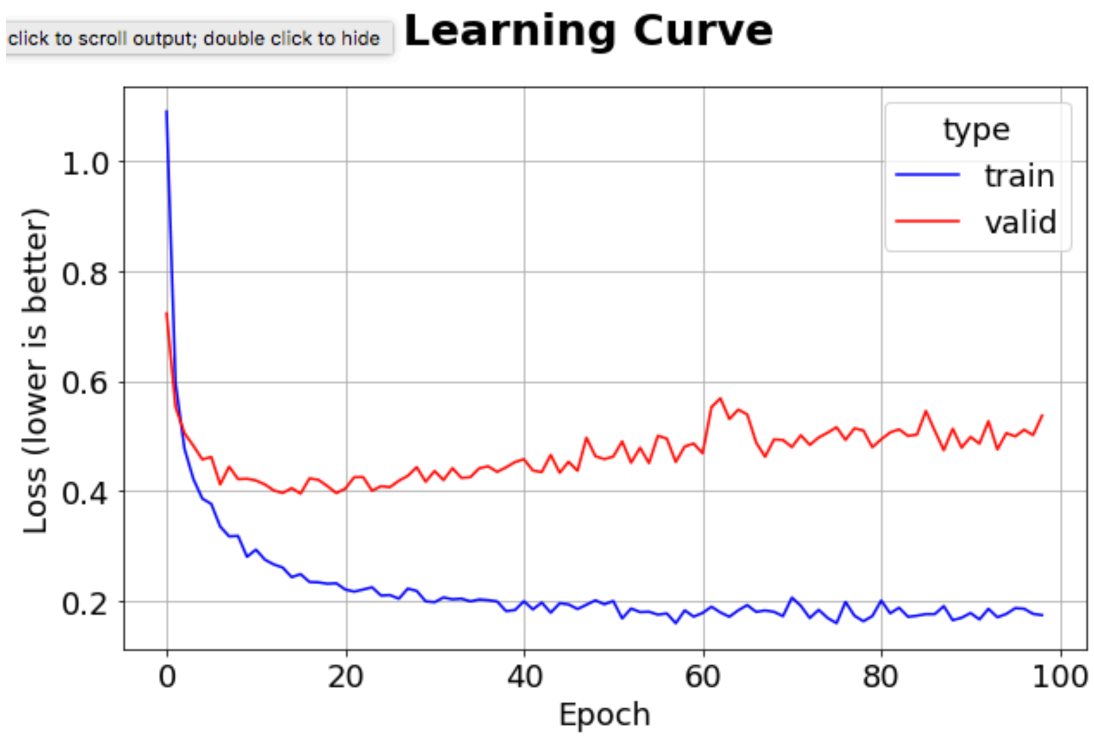


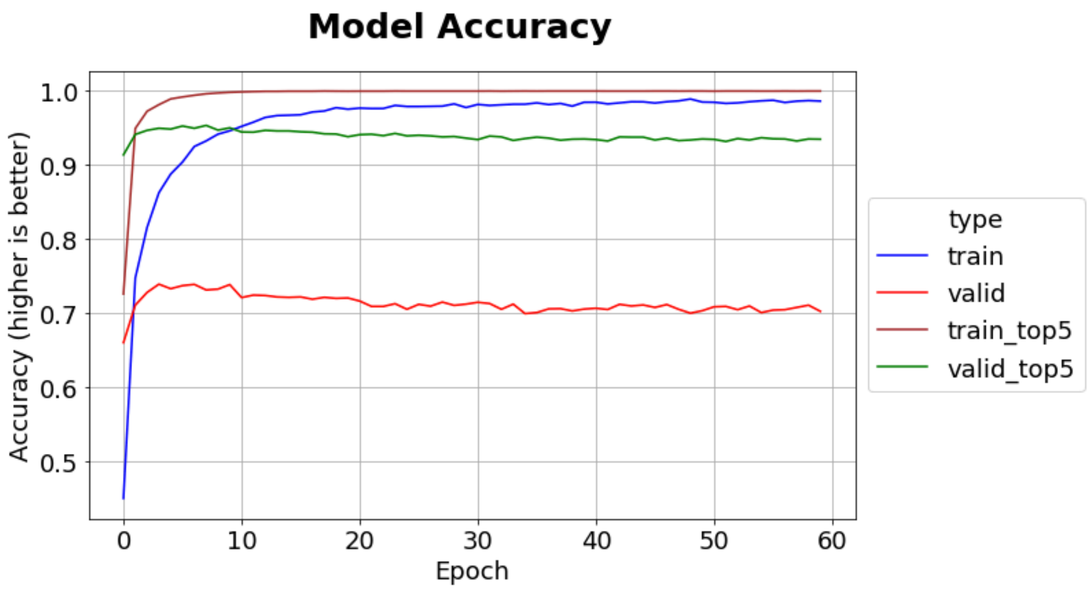
Flower vgg19



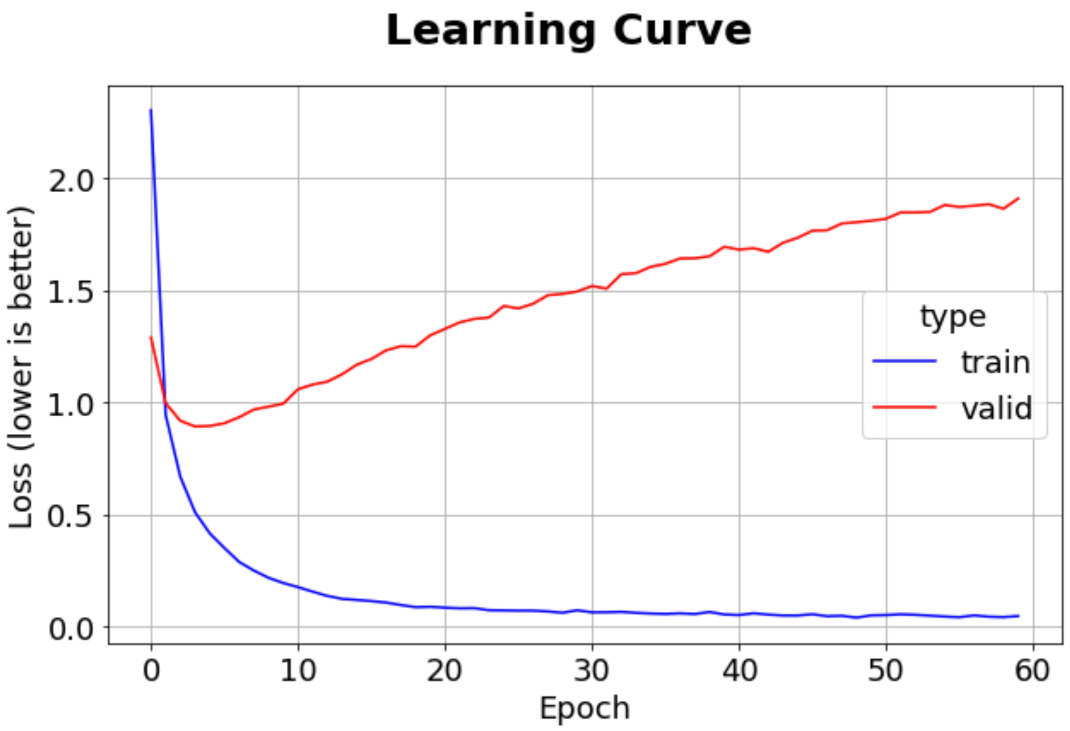


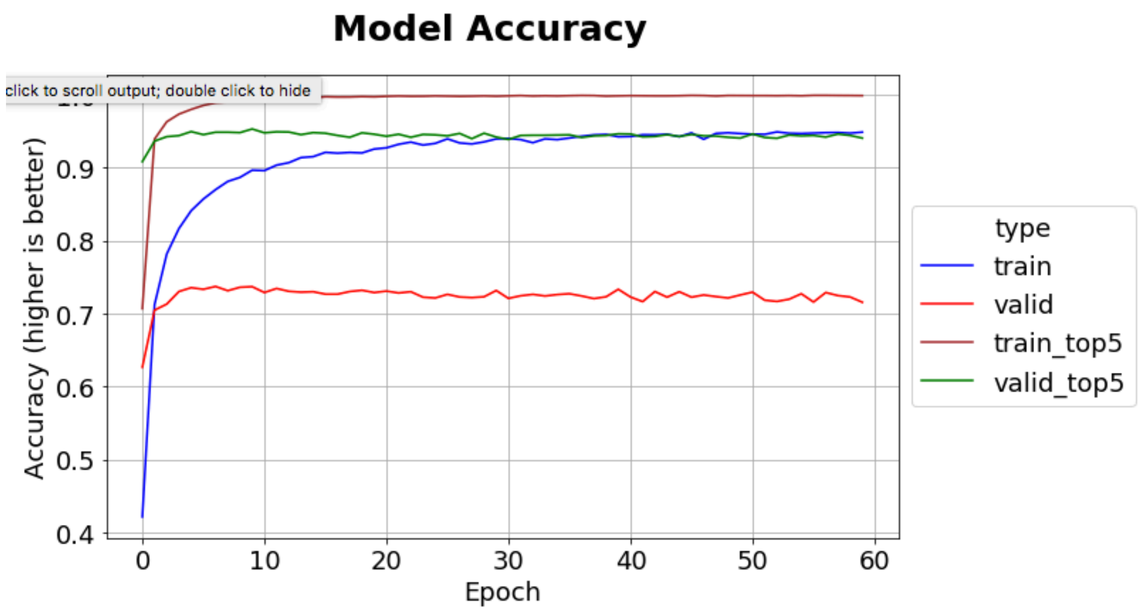
Flower da vgg19



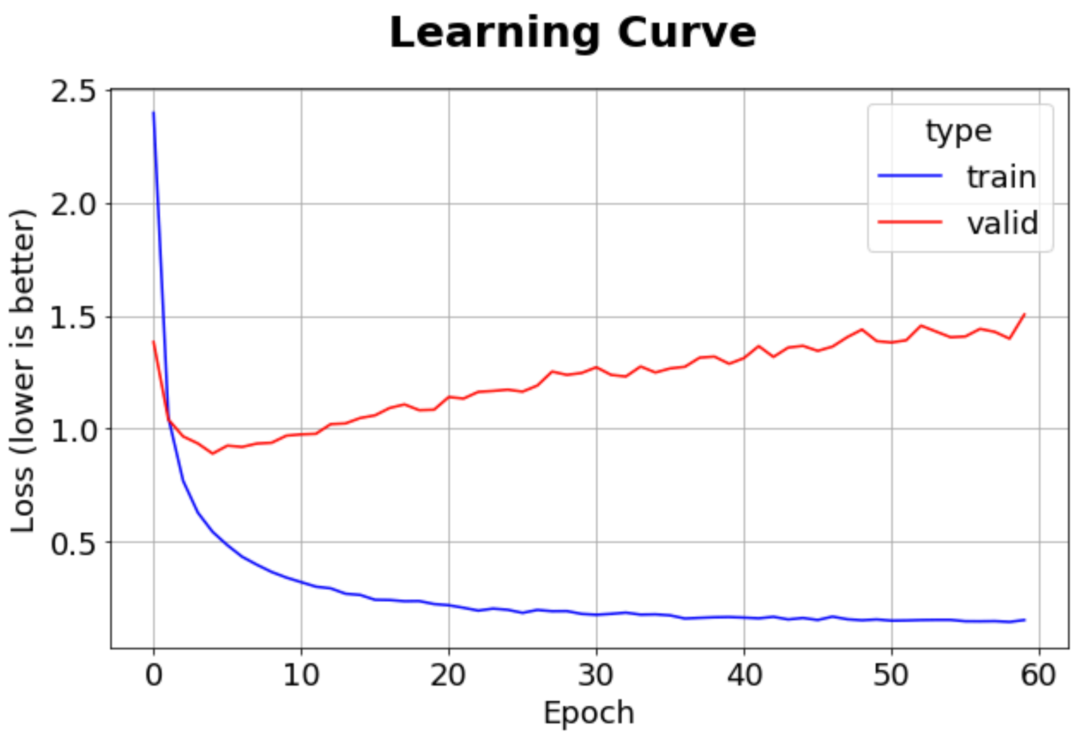


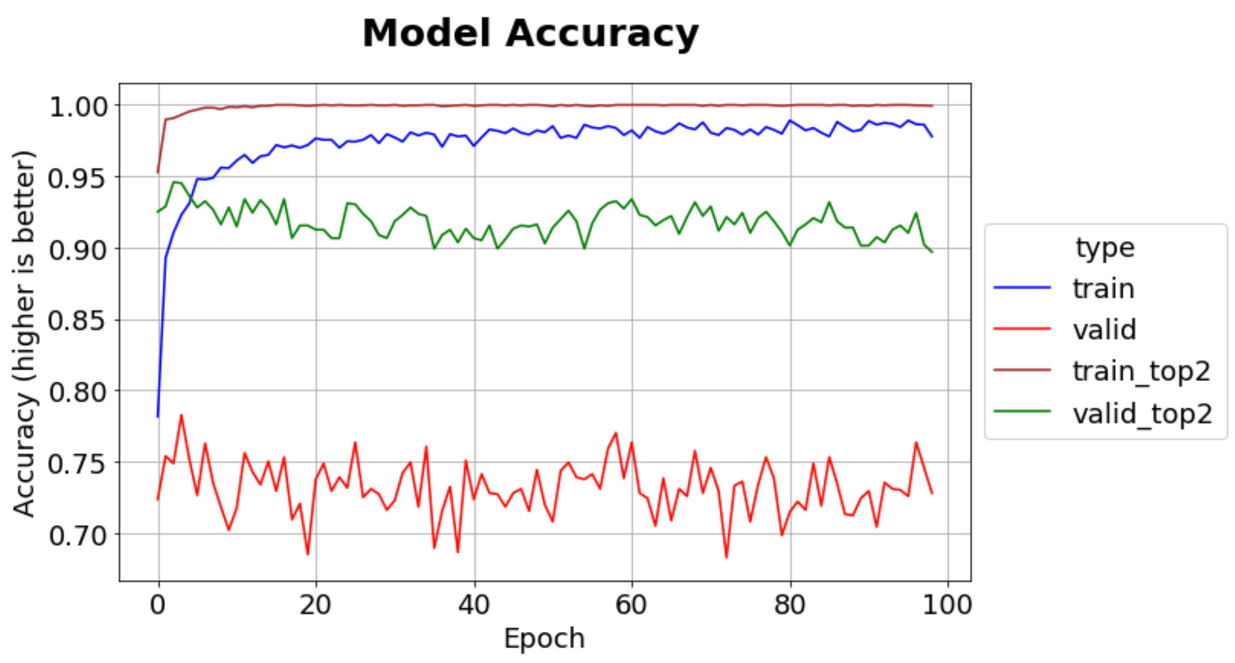
Stanford vgg19



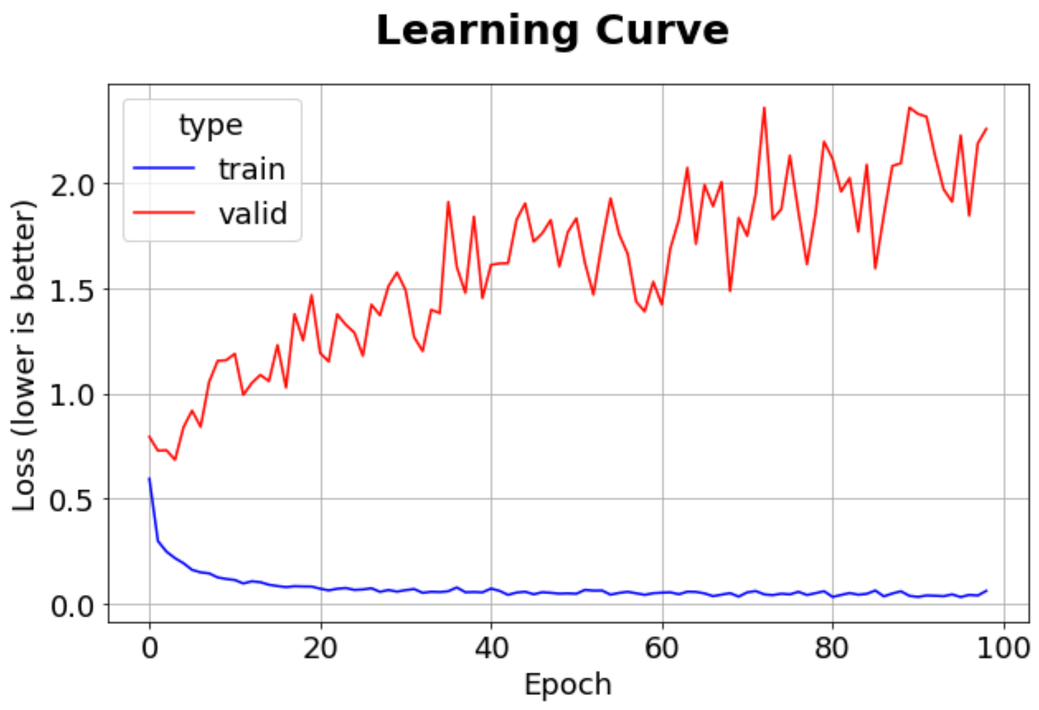


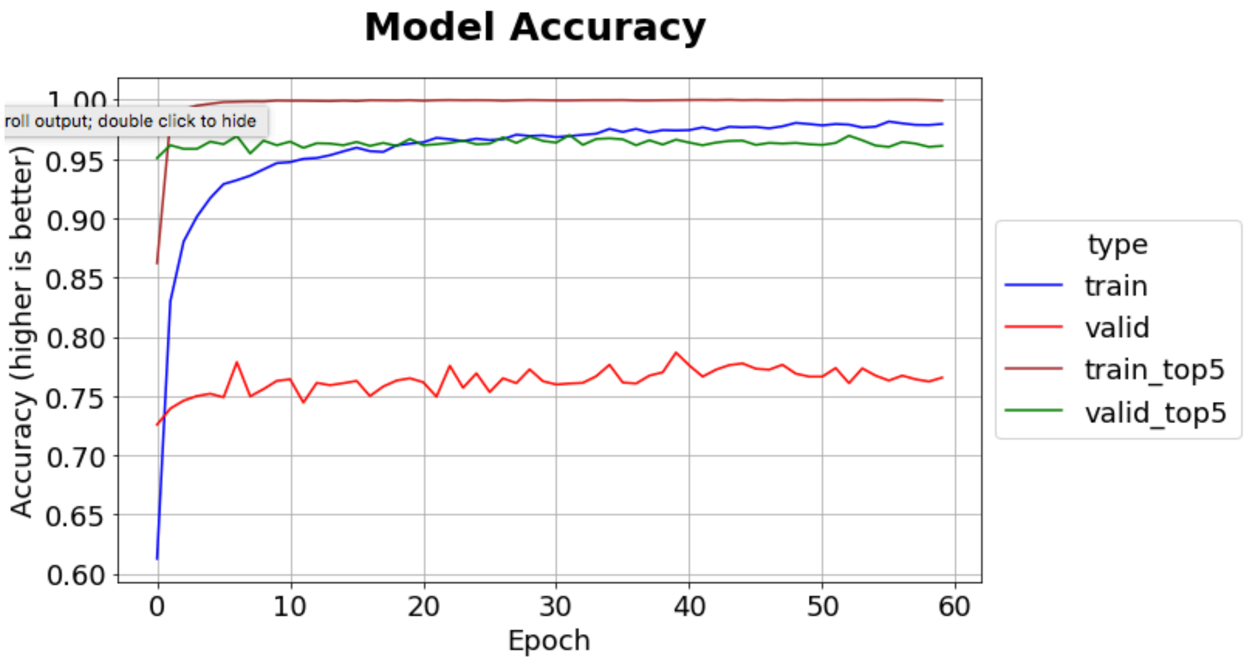
Stanford da vgg19



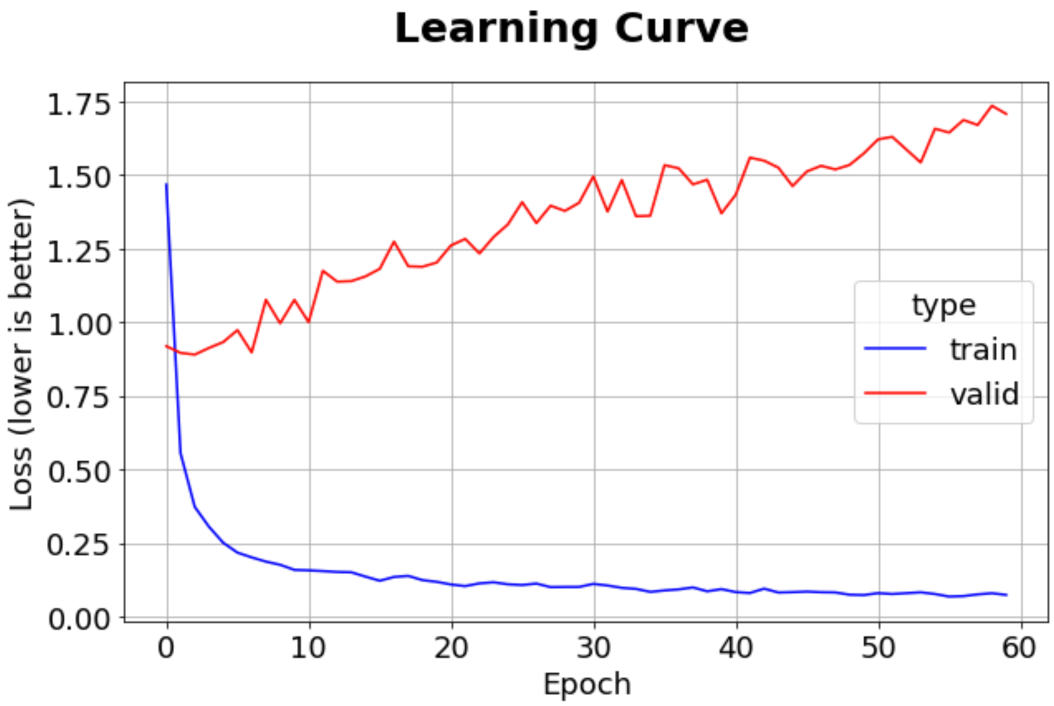


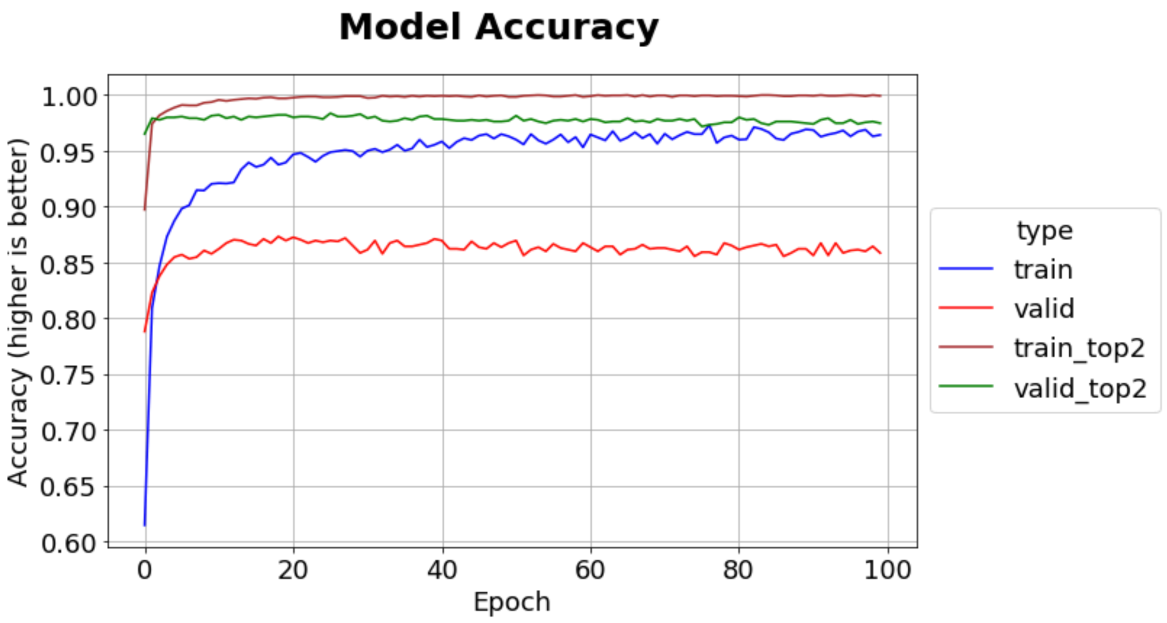
Flower_da_resnet



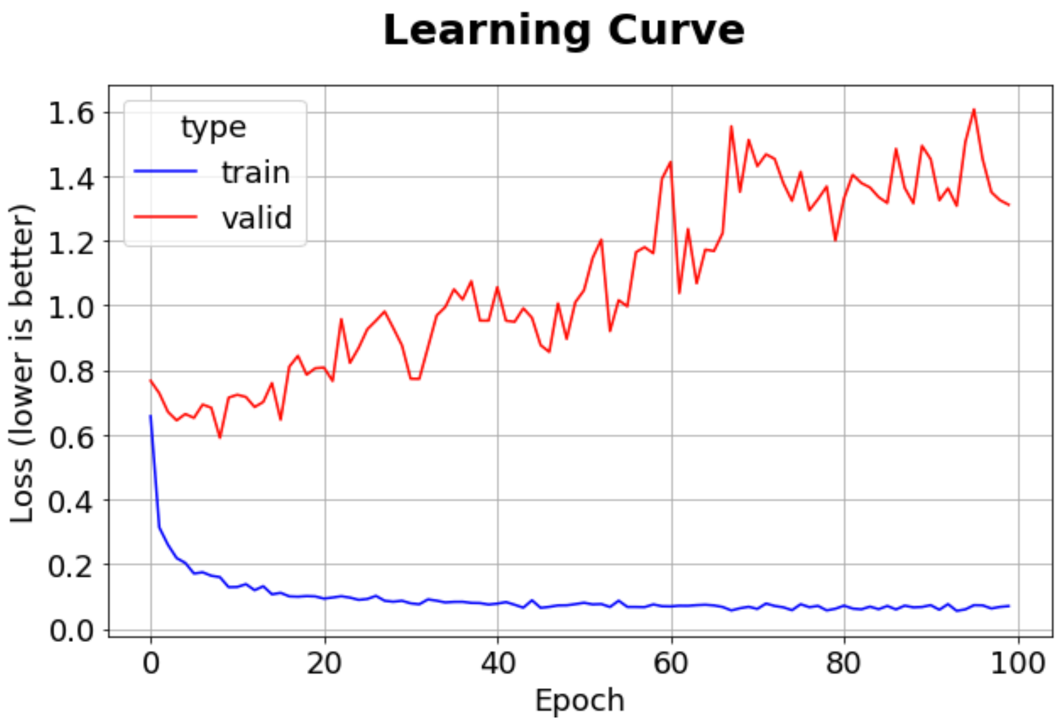


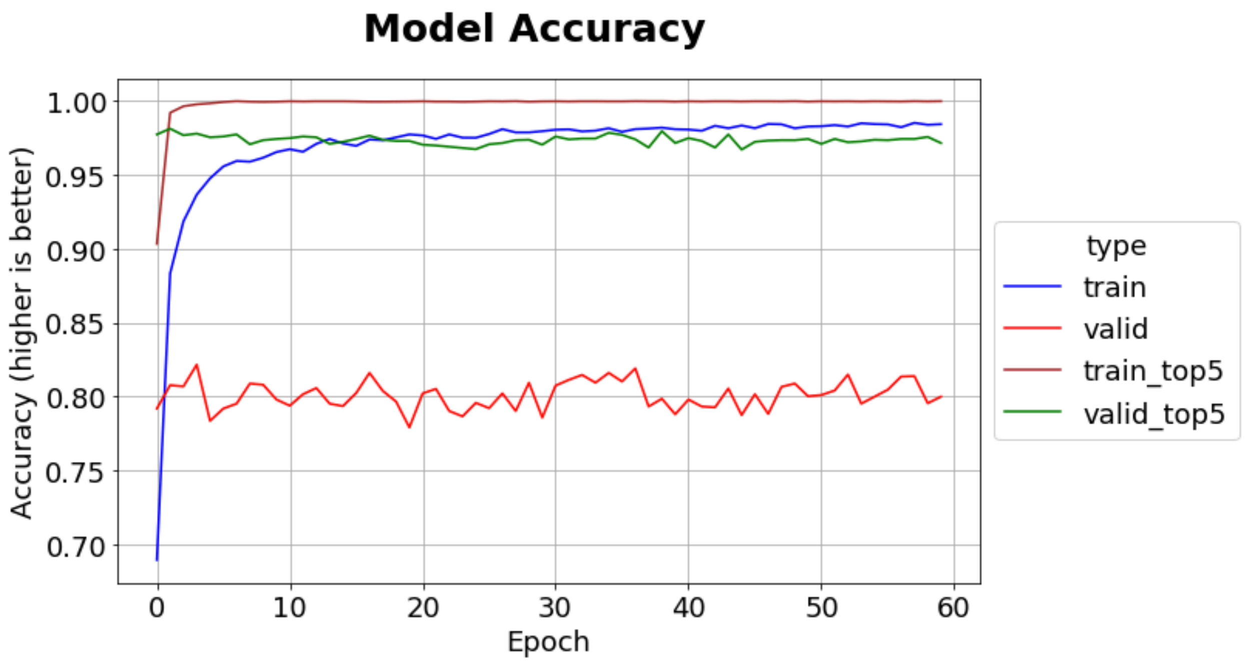
Stanford da Resnet50



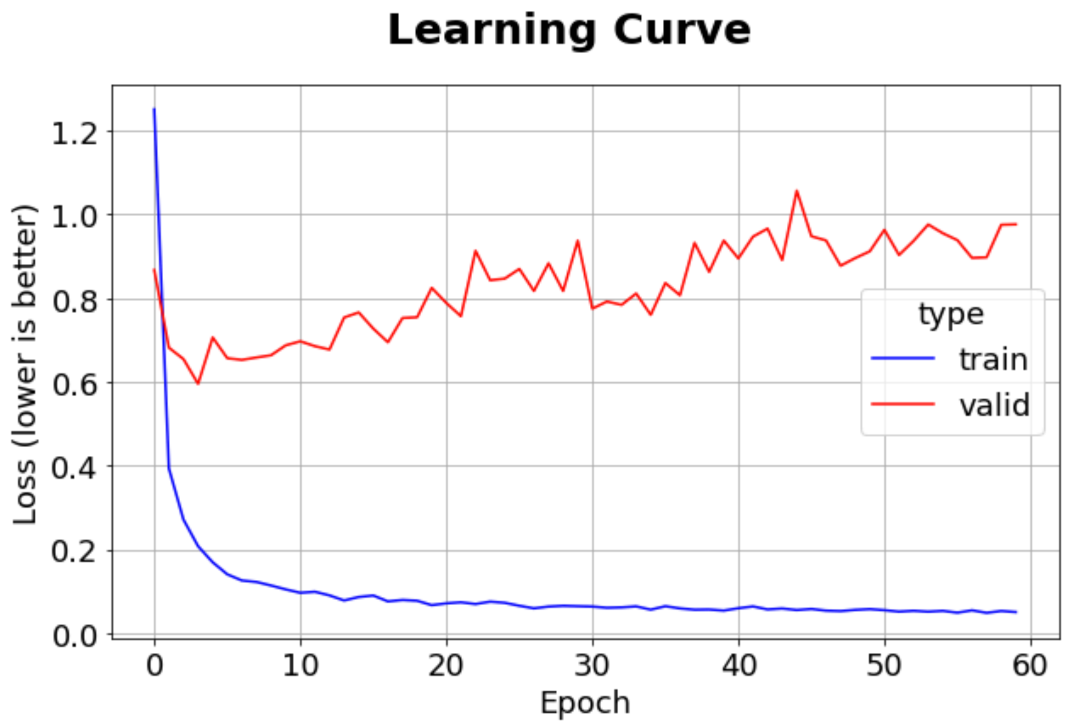


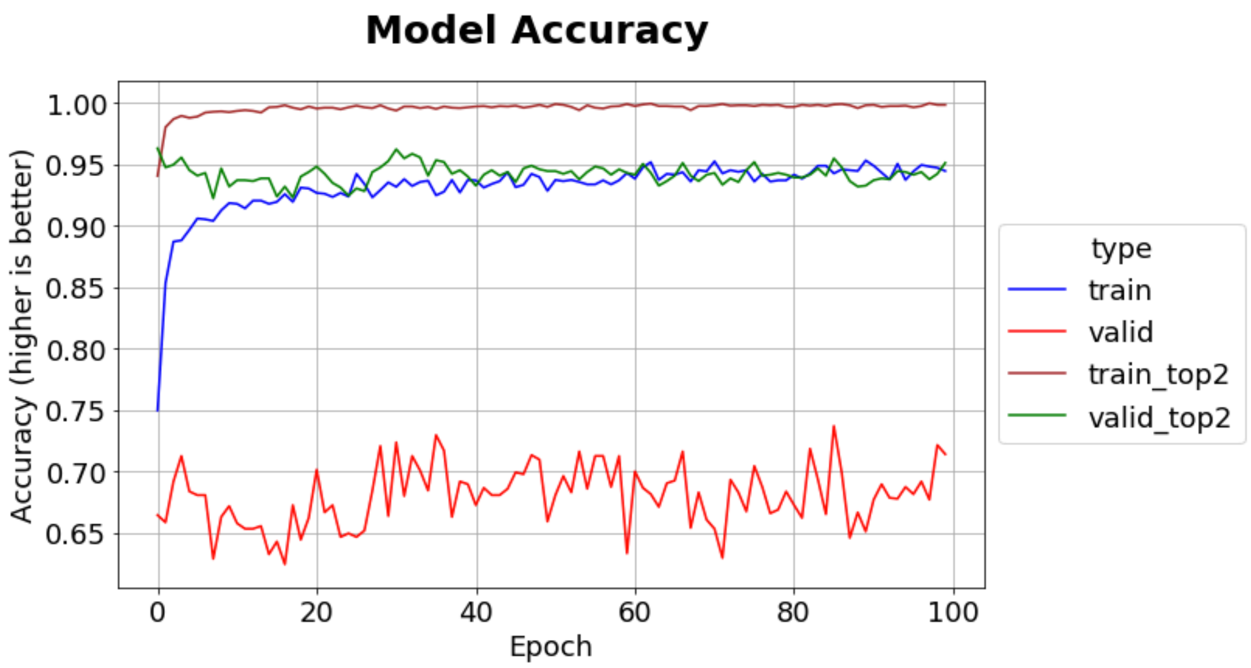
Flowers DA Densenet201



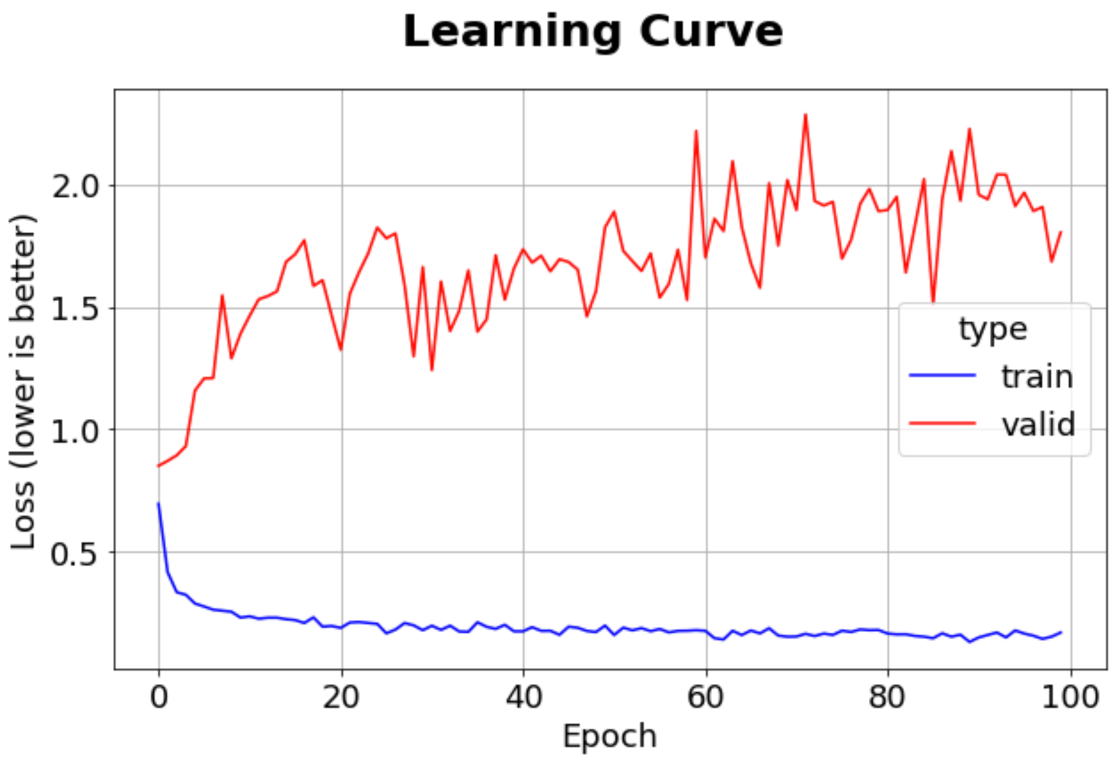


Stanford da DenseNet201





Flowers da inceptionV3



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note – identical references differentiated with *

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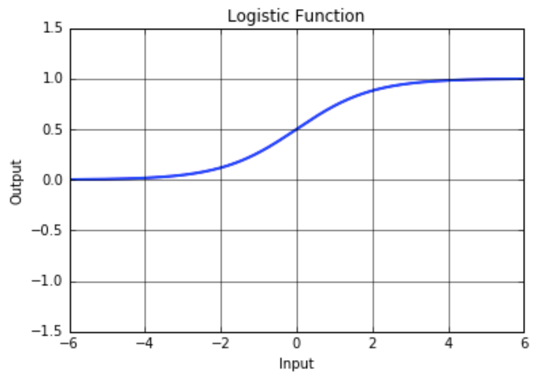
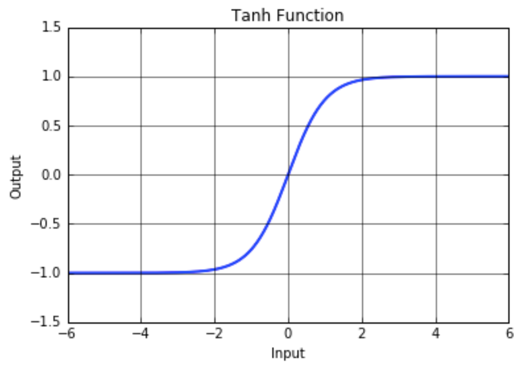
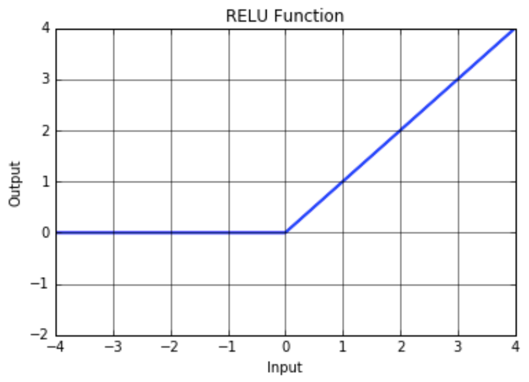
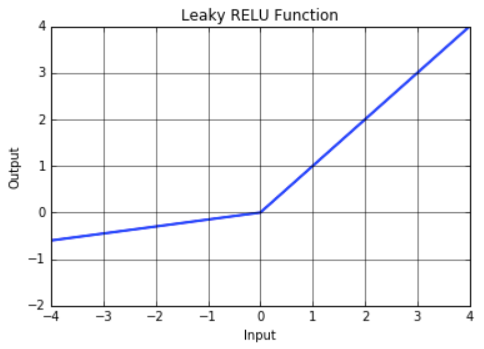
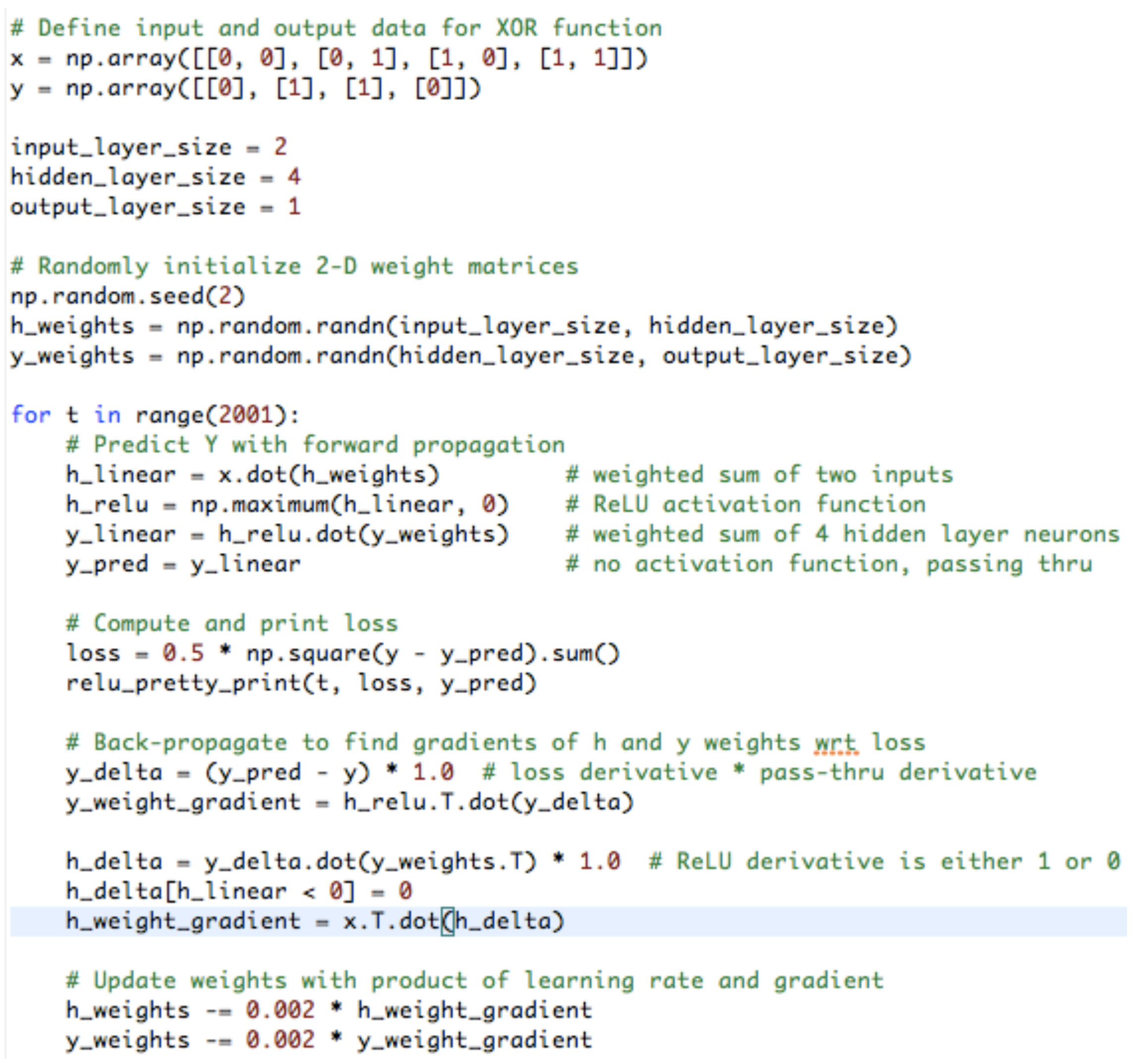
Appendix

	$Y = \frac{1}{1+e^{-x}}$ $Y' = Y * (1 - Y)$
	$Y = \frac{e^x - e^{-x}}{e^x + e^{-x}}$ $Y' = 1 - Y^2$
	$Y = x * (x > 0)$ $Y' = 1 * (x > 0)$
	$Y = x * \left(0.15 * (x < 0) + (x > 0)\right)$ $Y' = 0.15 * (x < 0) + 1 * (x > 0)$



```
# 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
```