Final Report: Reversible Architectures for Arbitrarily Deep Residual Neural Networks

Course 049064: Variational Methods in Image Processing

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Background

Deep Residual Networks as of recently have been pushing state-of-the-art performance tasks with deeper and wider architectures. This paper has set out to interpret Deep Residual Networks as ordinary differential equations (ODEs). The motivation behind this, is the fact that ODEs have long been studied in mathematics and physics with rich theoretical and empirical success. Using this interpretation, the authors developed a theoretical framework on stability and reversibility of deep neural networks, the paper outlines three reversible neural network architectures that may go arbitrarily deep in theory.

The backbone of this paper is in proving the reversibility of the networks, which in turn allow for memory-efficient implementations, as they have no need to store the activation functions for most of the layers

The paper goes into detail of the theoretical background (which we will cover in this section) and demonstrates examples of experiments done, which we will replicate and improve on. Datasets used in the experiments are CIFAR-10, CIFAR-100, and STL-10. With baseline architectures used as comparisons. A major strength of the paper's implementation is that the models built using the theoretical background out perform strong baseline models, over fewer training data.

The authors claim the problem with Residual Networks is that, although widely used, there exist little theoretical analysis and guidelines for designing and training ResNets. This can be solved by viewing ResNets as ODEs as follows:

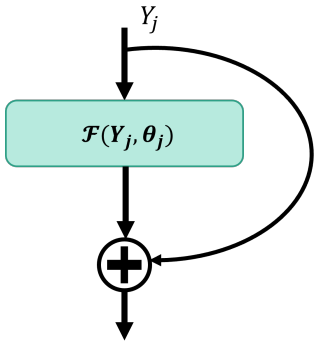


Figure 1: residual block

Output of block:

$$Y_{j+1} = Y_j + \mathcal{F}(Y_j, \theta_j)$$

multiply by h

$$Y_{j+1} = Y_j + h\mathcal{F}(Y_j, \theta_j) \rightarrow$$

$$\mathcal{F}(Y_j, \theta_j) = \frac{Y_{j+1} - Y_j}{h}$$

$$\xrightarrow{h \to 0}$$

$$\boxed{\dot{Y}(t) = \mathcal{F}(Y(t), \theta(t)); \quad Y(0) = Y_0} \tag{1}$$

A important definition to outline is "Reversibility", as it is the key element which allows for memory efficient implementations.

Definition Reversibility: An architecture is reversible if it allows the reconstruction of the activations going from the end to the beginning.

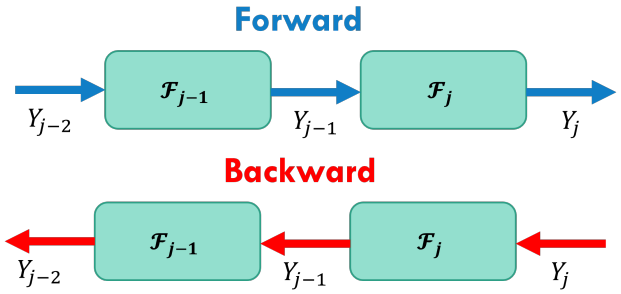


Figure 2: forward and backward diagram

A network is reversible if for:

$$Y_{j-2} = \mathcal{F}_{j-1}^{-1}(\mathcal{F}_j^{-1}(\dots \mathcal{F}_N^{-1}(Y_N)))$$
$$Y_j = \mathcal{F}_j(\mathcal{F}_{j-1}(\dots \mathcal{F}_N(Y_0)))$$
$\mathcal{F}_k^{-1}$ Exists $\forall k \Rightarrow$ Architecture is Reversible

Understanding how reversibility allows for a memory efficient implementations will be explored through an example further on, under the Section "Single Problem"

Another definition which is important to understand, which is derived from the realm of ODEs, stability. It is imortant to note that not every method that is algebraically reversible is numerically stable.

Definition Stability: A dynamical system is stable if a small change in the input data leads to a small change in the final result.

To further better characterize this, assume a small perturbation, $\delta Y(0)$ to the initial data $Y(0)$, assume this change is propagated throughout the network. The question is, what would be the change after some time t, that is what is $\delta Y(t)$? This change can be characterized by the Lyapunov exponent (λ):

$$\|\delta Y(t)\| \approx e^{\lambda t} \|\delta Y(0)\|$$

For a system, the "Forward Propagation" is well-posed (stable) when $\lambda \leq 0$, and ill-posed (unstable) if $\lambda > 0$.
It is easy to determine λ, as a bound on λ can be derived from the eigenvalues of the Jacobian matrix of $\mathcal{F}$ with respect to Y, which is given by:

$$J(t) = \nabla_{Y(t)} \mathcal{F}(Y(t))$$

A sufficient condition for stability is:

$$\boxed{\max_{i=1,2,\dots,n} Re(\lambda_i(J(t))) \leq 0, \quad \forall t \in [0,T]} \tag{2}$$

where $\lambda_i(J)$ is the ith eigenvalue of J, and $Re(\cdot)$ denotes the real part

Something the authors wanted to emphasis, the stability of the forward propagation is necessary to obtain stable networks that generalize well, but not sufficient. For a too small λ the networks decay too quickly are not able to learn. This is why the authors suggest selecting networks with a negative *lambda* ≈ 0

Previous Solutions

A paper titled "The reversible residual network: Backpropagation without storing activations" [1], does similar work to this paper. Though the approach in the competing paper, set out to put limitations on the activation layer, that allow for the network to be reversible. Our paper in contrast, put no such limitations and instead chose to approach a solution the problem as layed out in the previous chapter through the use of ODEs.

Another famous paper which improves upon ResNet, is the famous ResNxt network. Published in the paper "Aggregated residual transformations for deep neural networks" [2]. ResNxt introduces a homogeneous, multi-branch architecture to increase the accuracy.

Lastly worth mentioning is a paper titled "Deep networks with stochastic depth" [3], which reduces the training time while increasing accuracy by randomly dropping a subset of layers and bypassing them with identity functions (similar to ResNet).

Suggested Model

The authors present three different models in their paper:

- **Two-layer Hamiltonian Networks**
- **Midpoint Network**
- **Leapfrog Network**

We will start by presenting the model we chose to present, implement and improve upon. This model's architecture is inspired by Hamiltonian systems

$$\dot{Y}(t) = \sigma(K(t)Z(t) + b(t))$$
$$\dot{Z}(t) = -\sigma(K(t)^T Y(t) + b(t))$$

$Y(t)$ and $Z(t)$ are partitions of the features, σ is an activation function, and the network parameters are $\theta = (K, b)$. For convolutional neural networks $K(t)$ and $K^T(t)$ are convolutional operators. It can be shown that the Jacobian matrix of this ODE satisfies the condition of Ep.(2), leading to the conclusion that this network is stable and well-posed. The original Hamiltonian network [4] was designed using a single network. The authors claimed this was a limiting factor as the representability of a "single-layer" didn't generate satisfactory results. There for a "two-layer" architecture was suggested, which is what was used in the experimentation phase. The "two-layer" Hamiltonian equations are:

$$\begin{aligned} \dot{Y}(t) &= K_1^T(t)\sigma(K_1(t)Z(t) + b_1(t)) \\ \dot{Z}(t) &= -K_2^T(t)\sigma(K_2(t)Y(t) + b_2(t)) \end{aligned} \tag{3}$$

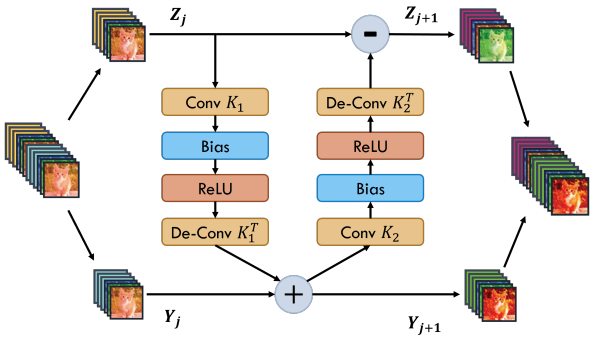


Figure 3: Two-Layer Hamiltonian

In discrete form (acquired using the Verlet method):

$$Y_{j+1} = Y_j + hK_{j,1}^T\sigma(K_{j,1}Z_j + b_{j,1}))$$
$$Z_{j+1} = Z_j - hK_{j,2}^T\sigma(K_{j,2}Y_{j+1} + b_{j,2}))$$

We will present a brief explanation of each of the other models. For the **Midpoint Network** the basis for it's model lays in the numerical method for discretization of the ODE as described in Eq.(1), done by using a central finite differences in time method:

$$\frac{Y_{j+1} - Y_{j-1}}{2h} = \mathcal{F}(Y_j)$$

Gives the following forward propagation

$$Y_{j+1} = Y_{j-1} + 2h\mathcal{F}(Y_j), \quad \text{for } j = 1, \ldots, N-1$$

The last model presented in the paper is the **Leapfrog Network**, which simply put is a special case of the Hamiltonian network Eq. (3), where one of the kernels is the identity matrix and one of the activations is the identity function. The leapfrog network involves two derivatives in time and reads

$$\ddot{Y}(t) \approx h^{-2}(Y_{j+1} - 2Y_j + Y_{j-1})$$
$$\xrightarrow{\text{Discrete Form}}$$
$$Y_{j+1} = \begin{cases} 2Y_j - h^2K_j^T\sigma(K_jY_j + b_j), & j = 1 \\ 2Y_j - Y_{j-1} - h^2K_j^T\sigma(K_jY_j + b_j), & j > 0 \end{cases}$$

Diagrams of Midpoint Network and Leapfrog Network blocks

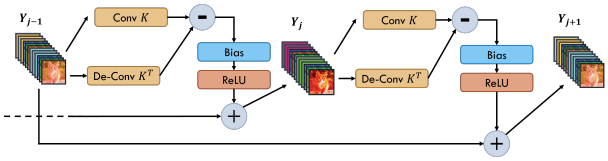


Figure 4: Midpoint Network Block

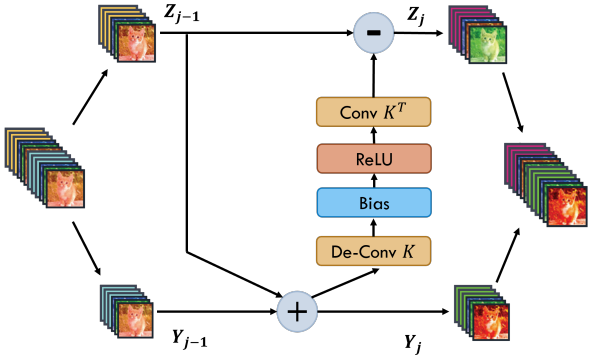
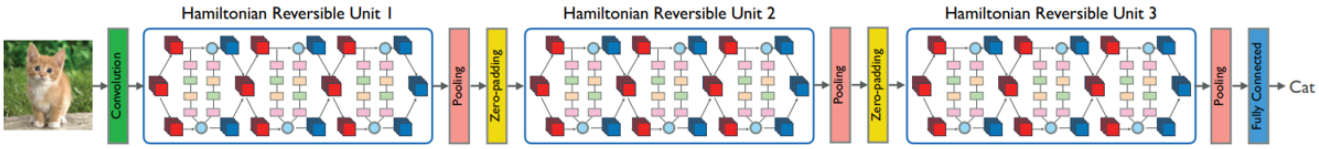


Figure 5: Leapfrog Network Block

The blocks a chained together to make a neural network as depicted in the following diagram (Hamiltonian Network)



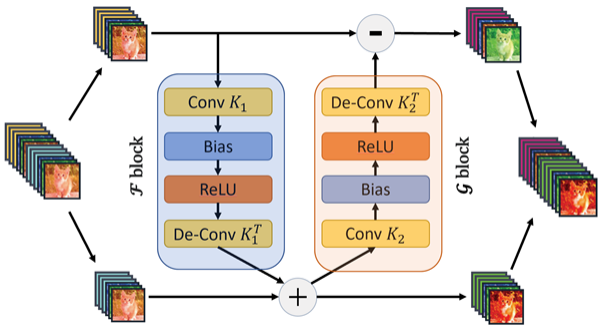
Implementation

We decided to implement the double layered Hamiltonian architecture. The writers of the paper implemented the model on MATLAB, without using the Deep Learning toolboxes that MATLAB provides. Our impression of the writer's implementation was that the code is hard to understand, and the code structure is confusing. In addition, their implementation relies on CudNN libraries that are not available for all. Due to all these factors we decided to implement the model with Python using the PyTorch library [5]. PyTorch is an open-source machine learning framework that builds deep neural networks on a tape-based automatic differentiation system (auto-grad).

We will now go through the building stages of the model's framework, one module at a time, and understand each module's role in the model.

First, we start by implementing the Residual Functions, i.e., the $\mathcal{F}, \mathcal{G}$ blocks that are used in a reversible Hamiltonian block. The Residual Functions consist of a **convolutional layer** with a **bias term**, an **activation layer** (the paper suggested a Rectified Linear Unit, or ReLU) and a **transposed convolutional** layer with the *same weights* as the convolutional layer (in the paper the convolutional weights are described by the matrix K). For the convolutional and transpose convolutional layers to share weights, we implemented the forward pass using Pytorch's functionals, inputting the same weight parameters for the convolution and transpose convolution functional.

The next module we implemented is the Reversible Hamiltonian Block, that is built using two Residual Functions ($\mathcal{F}$ block and $\mathcal{G}$ block) with the following architecture:



To implement the minus sign at the end of the $\mathcal{G}$ block we added support in the Residual Function module with a field called 'sign' that takes values of $\{1, -1\}$ and multiplies the tensor by that value before outputting from the block.

Back to the Reversible Hamiltonian Block implementation, the input tensor is split along the channel dimension into two equal groups (as suggested by the paper) and each group moves through the block as described in the figure above. At the end of the block the two groups are concatenated back into one tensor, and it is moved to the next block.

The backward pass of the Reversible Hamiltonian Block incorporates the blocks reversibility, using the tensor from the following block to restore the activations of the current block. We carefully deleted any unused variables so now unused memory was stored, stressing the advantages of memory efficiency of reversible architectures.

For the forward and backward passes of the Reversible Hamiltonian Block to be applied in the auto-grad framework, we implemented a **Reversible Unit Function** that wraps the forward and backward functions as static methods used by all reversible units.

Next, we implemented the Reversible Hamiltonian Unit, that is a sequence of several Reversible Hamiltonian Blocks chained together. The unit uses the Reversible Unit Function to apply forward and backward passes.

The Double layered Hamiltonian Network is comprised out of 3 Reversible Hamiltonian units, with average pooling between each layer. In addition, a convolution layer is added before the first unit and a fully connected layer is added to the output of the final unit. After each Reversible Hamiltonian Unit, the number of channels is doubled using zero padding.

In addition, we implemented the **weight smoothness decay regularization** in the PyTorch framework. This type of regularization is not supported by the default PyTorch optimizers and losses, therefore we were required to write a custom regularization function that computed the weight smoothness regularization term. The weight smoothness is calculated by penalizing the difference between the current weights and the weights before the optimizer step $\Sigma \|W_j - W_{j-1}\|_F^2$. We defined a weight cache to store the weights from the previous state (before the optimization step).

For training we used the hyper-parameters suggested by the paper: initial learning rate of 0.01, batch size of 128, momentum of 0.9, weight decay of $2 \cdot 10^{-4}$ and weight smoothness decay of $2 \cdot 10^{-4}$. The learning rate was decreased by a factor of 10 in epochs $80, 120, 160$. We trained on 200 epochs with validation steps every 20 epochs. We split the training data 10% for validation and the rest for training.

We performed our experiments using the CIFAR10[6] dataset on the Hamiltonian-218 network (18 Hamiltonian blocks per unit). We trained using a NVIDIA GeForce 2080 GPU that accelerated our training. Training time (when using the GPU) was approximately 27 seconds per epoch.

Analysis

Let us examine some of the results displayed in the paper. When examining the experimental results two main points jump out:

1. The accuracry of the suggested models perform poorly compared with the baseline models (on the CIF datasets)
2. The suggested models require significantly fewer parameters to train (as promised by the authors) and in turn perform better than the baseline models, on a subset of training data.

Name	Units	Channels	# Model Params (M)		Accuracy	
			CIFAR-10	CIFAR-100	CIFAR-10	CIFAR-100
ResNet-32	5-5-5	16-32-64	0.46	0.47	92.86%	70.05%
RevNet-38	3-3-3	32-64-112	0.46	0.48	92.76%	71.04%
Hamiltonian-74 (Ours)	6-6-6	32-64-112	0.43	0.44	92.76%	69.78%
MidPoint-26 (Ours)	4-4-4	32-64-112	0.50	0.51	91.16%	67.25%
Leapfrog-26 (Ours)	4-4-4	32-64-112	0.50	0.51	91.92%	69.14%
ResNet-110	18-18-18	16-32-64	1.73	1.73	94.26%	73.56%
RevNet-110	9-9-9	32-64-128	1.73	1.74	94.24%	74.60%
Hamiltonian-218 (Ours)	18-18-18	32-64-128	1.68	1.69	94.02%	73.89%
MidPoint-62 (Ours)	10-10-10	32-64-128	1.78	1.79	92.76%	70.98%
Leapfrog-62 (Ours)	10-10-10	32-64-128	1.78	1.79	93.40%	72.28%
ResNet-1202	200-200-200	32-64-128	19.4	-	92.07%	-
Hamiltonian-1202 (Ours)	100-100-100	32-64-128	9.70	-	93.84%	-

Figure 6: Poor performance (Red), On par performance (Yellow), Superior performance (Green). Fewer Parameters (Violet)

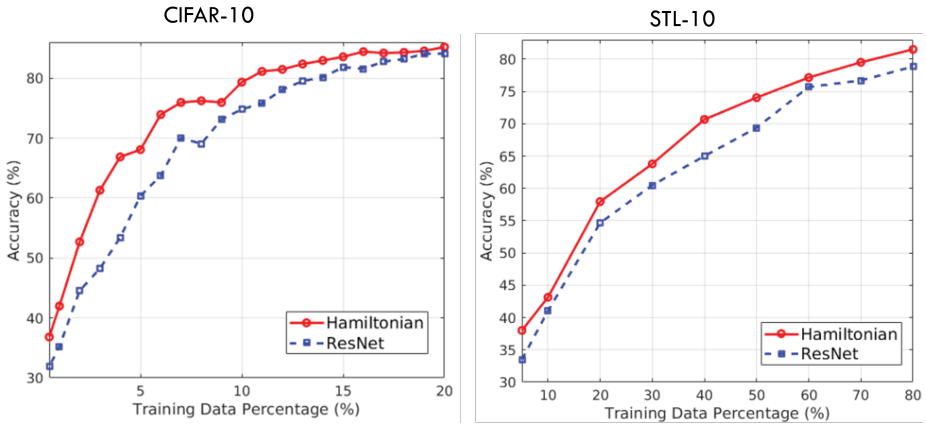


Figure 7: Both on CIFAR and STL datasets we set how the Hamiltonian network outperforms for "small" datasets (subset is % complete dataset)

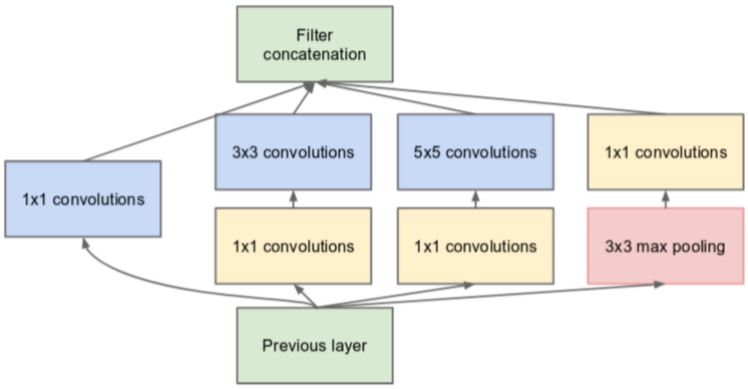
We selected the Hamiltonian Network as the model to further investigate, as it seemed to be the most mentioned in the paper. With it being the most experimented on, and most data about it available. So gauging our implementation would have ample data to compare with.

Creative and Suggested Improvements

As noted in the Analysis section, there is much left to be desired with regard to accuracy of the models offered by the paper. We have decided to address this issue with two approaches. The first approach is adding batch normalization and dropout layers to tackle over-fitting we experienced during training the original model. The second improvement was adding "inception blocks" (first introduced in "Going deeper with Convolutions"[7]) to $\mathcal{F}$ and $\mathcal{G}$ blocks.

First we will explain the justification behind inception blocks.

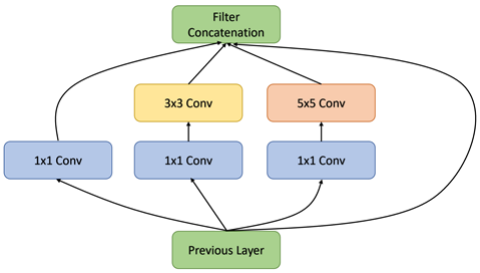
When designing a convolutional network, it is often difficult to select the best kernel size. Inception blocks seek to overcome this by incorporating several kernels of various sizes and applying them all at each stage. This has proven to be effective. The models tend to go "wider" (authors terminology) and require more computations, but improve the accuracy of the network. For us to be able to include these inception blocks in a Two-Layer Hamiltonian network for example, we must first prove that neither of the assumptions the Hamiltonian network guarantees, are violated. We will prove both "reversibility" and "stability" still apply to our model.



Two-Layer Hamiltonian-Inception Block:

$$Y_{j+1} = Y_j + hK_{j,1}^T \sigma(K_{j,1} Z_j + b_{j,1}))$$
$$Z_{j+1} = Z_j - hK_{j,2}^T \sigma(K_{j,2} Y_{j+1} + b_{j,2}))$$

Here we will present the proof that the inception block can be represented as a kernel K. This would in turn show the model with inception blocks to be: 1) Stable, 2) Reversible
We use the following block in our model:



1×1, 3×3, 5×5 are convolution operators with kernel sizes $1, 3, 5$ and the filter concatenation is an element wise summation of the output channels.
Notice here we implemented a variation of the inception block, which includes a skip connection (a linear operator).

Proof.
Convolutional operators are linear[8]

$$\forall A, B \text{ linear operators } \rightarrow AB = C \text{ is also a linear operator}$$

we know that a sum of linear operators are also a linear operator

$$\Rightarrow I(x) = C_{1\times1}x + C_{3\times3}C_{1\times1}x + C_{5\times5}C_{1\times1}x = (C_{1\times1} + C_{3\times3}C_{1\times1} + C_{5\times5}C_{1\times1})x$$
$$\Rightarrow I(x) = Kx$$

■

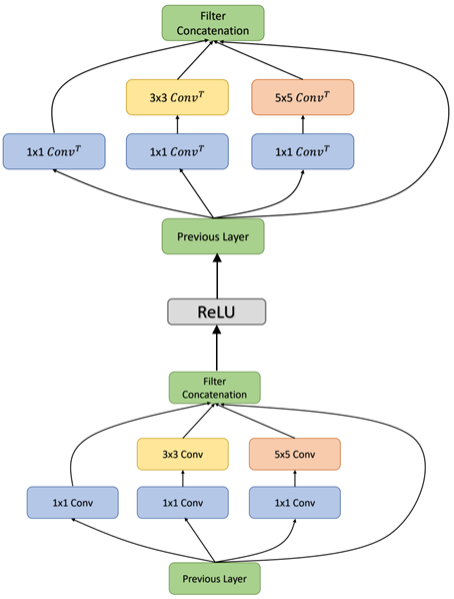
Back to our implementation.

For our first approach, we added batch normalization after the initial convolution layer and a dropout layer with factor 0.4 before the fully connected layer. These two regularization methods help tackle *overfitting* that we encountered during the training of the original architecture. Both methods are well known and are commonly used in deep neural networks. From our analysis they do not harm the reversibility and stability of the Hamiltonian blocks (as they are outside of the blocks) thus they promise to improve the results.

Batch normalization re-centers and re-scales each batch, smoothing the objective function and helping the optimization to find the global minima. Dropout layers are activated only during training. They "de-activate" neurons with a probability of a Bernoulli distribution with a factor p (in our case p=0.4). Dropout encourages the network to learn a sparse representation as a side-effect.

We trained the Regularized Hamiltonian Network in the same manner as the original network, with a difference of using $5 \cdot 10^{-4}$ weight decay.

The second improvement we added was adding inception to the $\mathcal{F}$ and $\mathcal{G}$ blocks. We did this by splitting the $\mathcal{F}$ or $\mathcal{G}$ block input into 4 groups. One was passed as a skip connection. The second was passed through a 1x1 convolution layer. The third was passed through a 1x1 and then 3x3 convolution layers and the last group was passed through 1x1 and then 5x5 convolution layers. Afterwards, the 4 groups were concatenated and continued to an activation layer (ReLU). Finally, the tensor was split again into 4 and the same process was done only with transpose convolution layers with shared weights to the initial convolution layers. At the end of the block the groups were concatenated, and the tensor continued its flow. The architecture is described in the following figure:



We trained the Inception Hamiltonian network on 250 epochs, with initial learning rate of 0.001 and weight decay of $5 \cdot 10^{-4}$. All the other hyper-parameters were the same as in the training of the original network. The training time for the Inception Hamiltonian network (while using a GPU) was approximately 48 seconds per epoch.

Presented here is a table with our final scores:

Model	Train Loss	Test Acc
Original Network	2.05	96%
Original Network + batch normalization & dropout	1.62	97%
Inception block Network	1.08	68%

First thing to stand out, is the low Test accuracy for our inception implementation. We spent many hours trying to asses and improve this, but our code is correct and the accuracy is accurate which leaves us with the conclusion, inception blocks don't always improve the model. While this was disappointing to discover, we want to note, we still were able to improve on the original authors models. Our network with dropout and batch-normalization, out performed the original model.
Progress of each model through the Training phase:

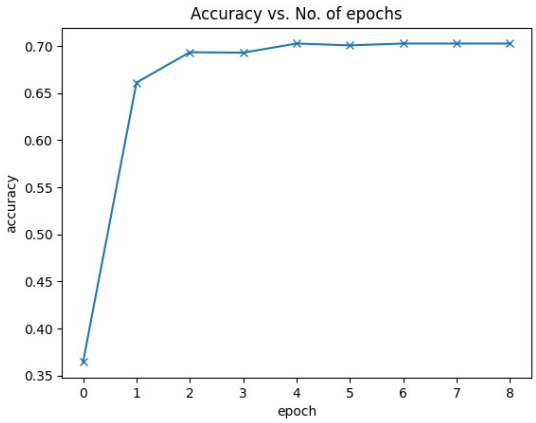


Figure 8: Accuracy - Original Model

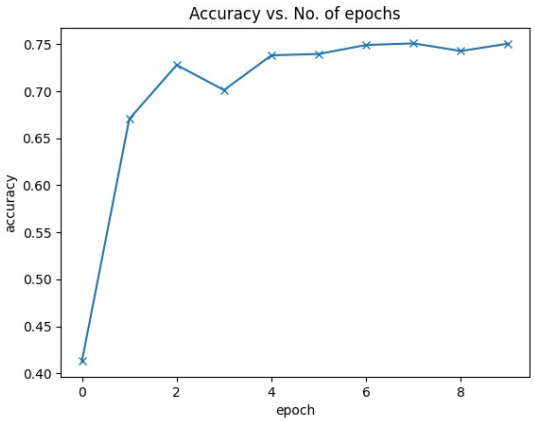


Figure 9: Accuracy - Model with dropout and batch-normalization added

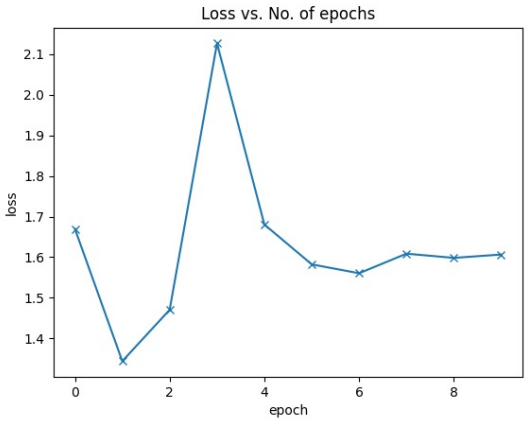


Figure 10: Loss - Model with dropout and batch-normalization added

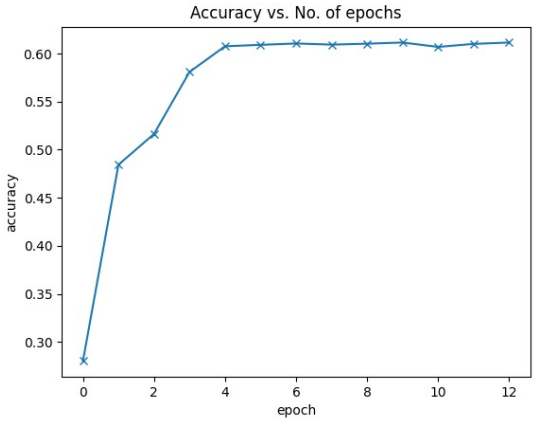


Figure 11: Accuracy - Model with dropout and batch-normalization added

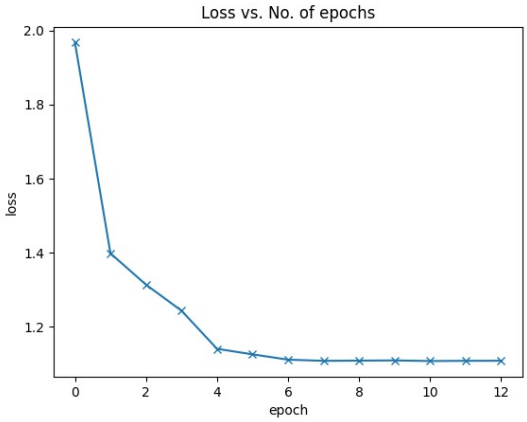


Figure 12: Loss - Model with dropout and batch-normalization added

Lastly a very important table which may offer a clue as to why the Inception Block performed so poorly.

	Original Network	Original Network + batch normalization & dropout	Inception block Network
Number of params	1,751,882	1,751,946	458,682

We can see a significant decrease in the number of parameters in the Inception block network, with the same amount of layers. Our conclusion is that perhaps the model did not have enough parameters to reach significant enough model.

Conclusion

We started this project with an idea in mind, we were unsure if it would succeed but talked at length about the different approaches we could take, and selected the one we felt was most promising. A lot of what we learned throughout the project was novel to us and required learning beyond the scope of the course. Implementation of the paper was no small task, our full repository can be found here: Github.

As mentioned early on we had a short correspondence with the authors of the paper, seeking their implementation. But their repository seemed lacking and not up to date. It was missing models and the code was not entirely consistent with the paper.

Researching DNN can be a bit tricky and in many cases it comes down to experimental data, attempting certain changes and noting a performance increase or decrease. While here in the final report we noted the improvements, they were not achieved immediately, and our model went through many unsuccessful iterations.

We feel satisfied with our final result, as it reached the goal of improving upon the original authors solution and did not degrade in any way the performance. Though it should be noted our original research question (can we improve the models by incorporating inception blocks?) did not meet expectations, while remaining within the frame of the paper.

Some future possibilities to further expand on, at the very basic level, develop improved models for the other models suggested by the authors (Leapfrog Network, Midpoint Network). Perhaps expand on some of our original ideas exploring other networks not suggested by the paper, using PDE's, including finding models with a higher order PDE. Though after a lengthy discussion we concluded most models suggested based on higher order PDE's would require numeric solutions which in turn would be difficult to prove stability as defined in the paper.
Lastly at the time of writing this summary we are running some final tests on a much larger inception network (the authors who published the inception blocked, recommended it only be used on very large networks. Though no details on what large meant.), with hopes that an increase in layers would in turn increase the number of parameters, but we would be comparing a more complex network with the original 218 layer one. Therefore comparison would not be an equal evaluation.

References

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