Clustering-Oriented Representation Learning in Neural Networks

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RLLab
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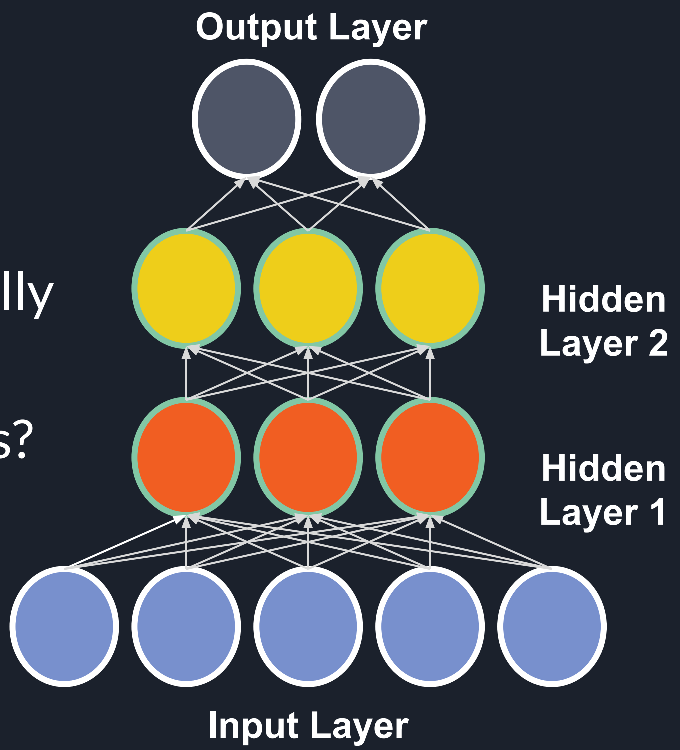
“The purpose of abstraction is not to be vague, but to create a **new semantic level** in which one can be absolutely precise.”
Dijkstra

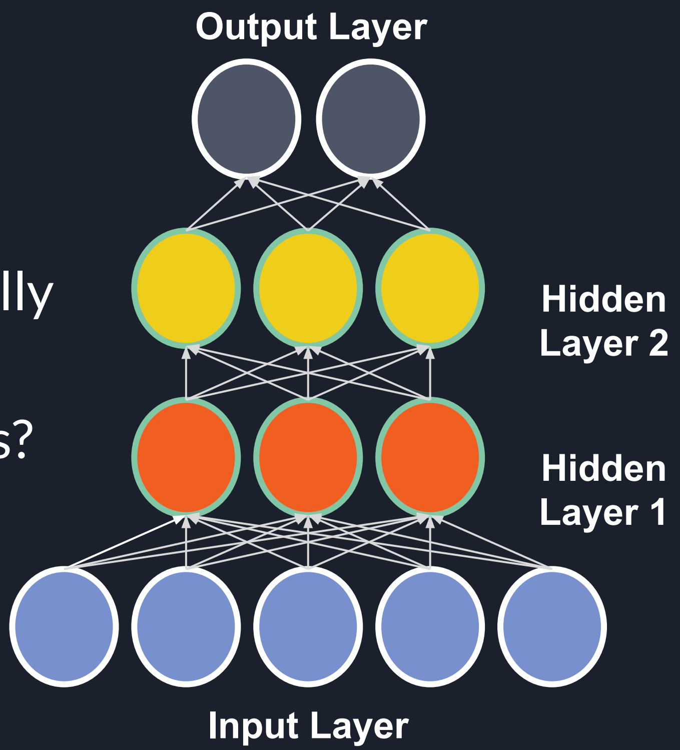
Neural Networks and Latent Representations

- What are the hidden layers in neural networks?
- Are they simply black boxes that magically solve problems, where we have no understanding of their internal workings?



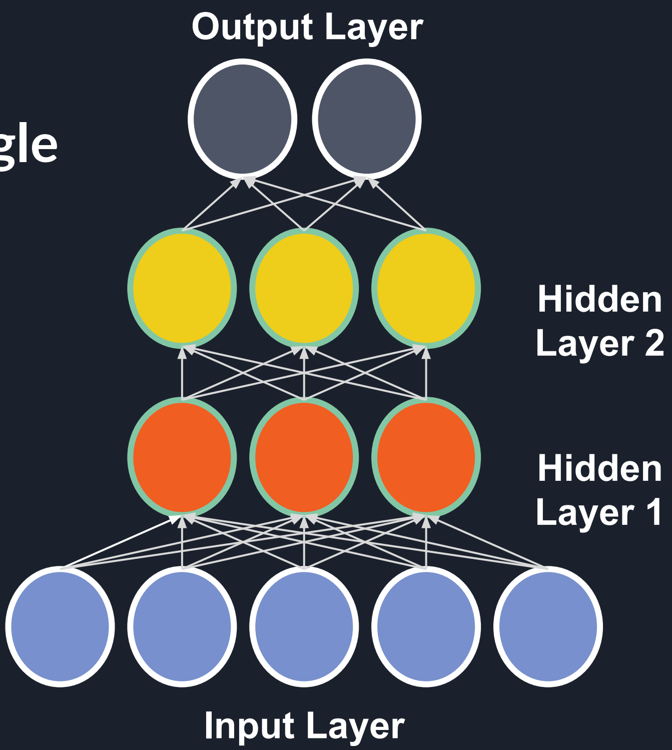
Neural Networks and Latent Representations

- What are the hidden layers in neural networks?
- Are they simply black boxes that magically solve problems, where we have no understanding of their internal workings?
- NO!

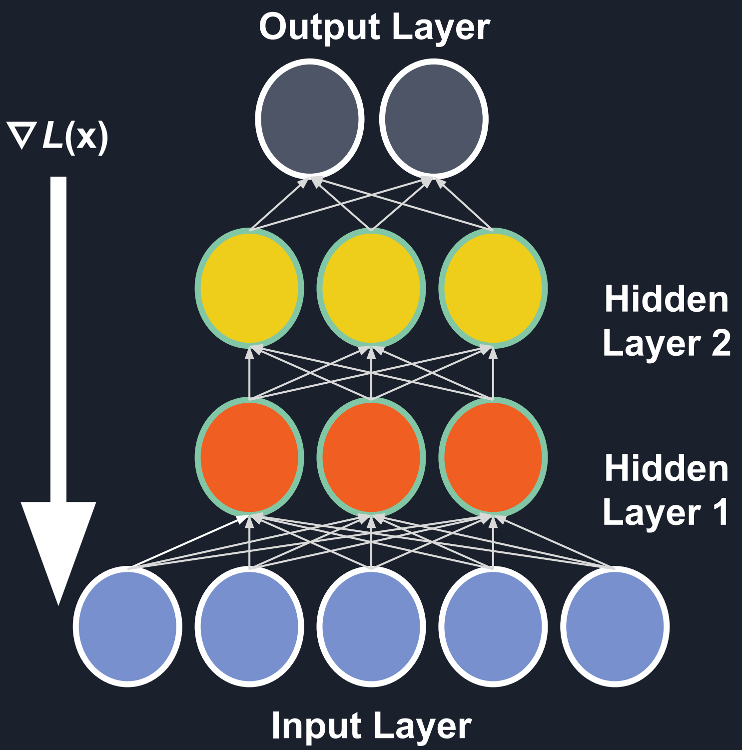


Neural Networks and Latent Representations

- Hidden layers are supposed to **disentangle the factors of variation in the data.**
- They use **nonlinear transformations** to project the data onto a new space with properties imposed by the loss function.
- The parameters of these nonlinear transformations are **learned with backpropagation**.



Neural Networks and Backpropagation



The usefulness of the hidden layers, and the properties they express, depends on the **loss function used to train the network**, the gradient of which is backpropagated through the network.

Categorical Cross Entropy Loss

- Categorical Cross Entropy is the standard loss function of a network designed for classification.
- Whereas logistic regression attempts to linearly separate the data in the **original feature space**, CCE in MLPs directly imposes the quality that the data should be linearly separable in a **new latent space**.

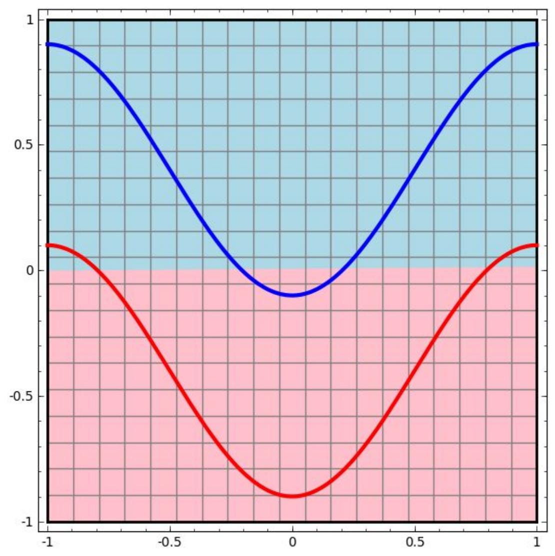
Linear Separability and Non-linear Transformations

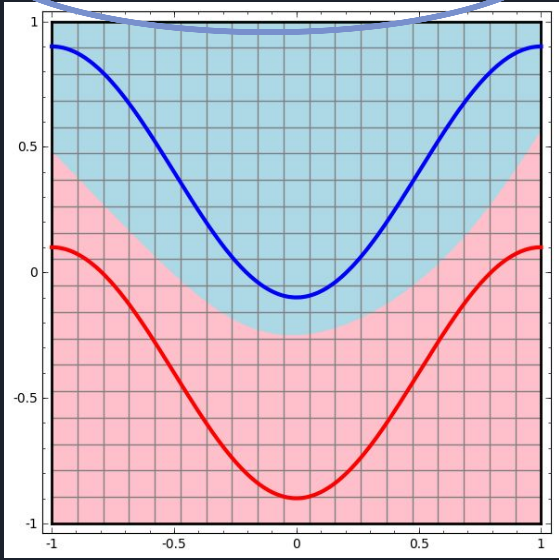
Same things, different views!

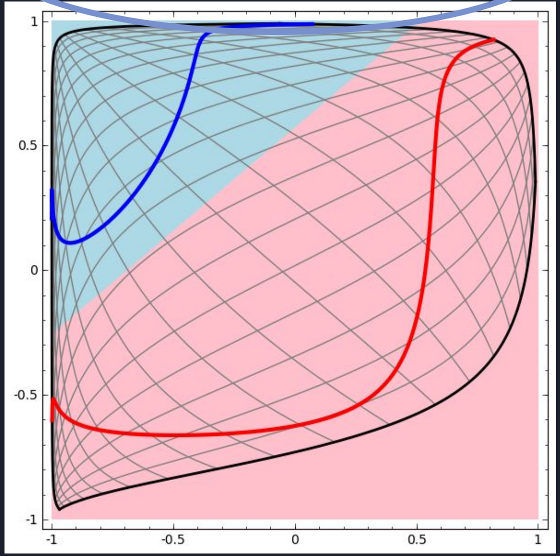
Linear Separation in Feature space, made by logistic regression. Not a perfect separation, and cannot be.

Non-Linear Separation in Feature space, made by neural net. But, this is actually a reflection of -->

The linear separation in the **learned latent space, the learned non-linear transformation of data.**







See: http://colah.github.io/posts/2014-03-NN-Manifolds-Topology/

Categorical Cross Entropy Loss

- Linear separability, in the latent space, is the fundamental geometric property expressed by CCE.
- My research questions:
    - *Can we make the latent space **more "interpretable"** with a more geometrically motivated loss function?*
    - *Do we even **need an output layer**? Do we need linear separation to have a nice model?*

Clusterability for Latent Representations

According to (Bengio et al., 2013), a desirable quality for our latent representations would be if they were **naturally clusterable**, that is that "different values of categorical variables such as object classes are *associated with separate manifolds*."

Clustering like it's 1957 (the year K-Means was theorized...)

- We would like impose "clusterability" with a new loss function, since CCE doesn't do so (it only imposes linear separability).
- Let's be like K-Means and use **centroids**!
- Not just any centroids, but **latent categorical centroids**...

Clustering like it's 1957 (the year K-Means was theorized...)

Latent Categorical Centroids:

- Each class *c* gets a latent categorical centroid, E_c :
  - $E_c = (1/|C|) \sum h(x_i)$
  - *For each sample x_i in C; e.g., belonging to class C.*
- In other words, E_c is the mean latent representation, *h(x)*, over all samples, x_i, for class *c*.

Clustering like it's 2017... With Neural Networks!

- Now, if we have K classes in our dataset, we can construct K centroids, $E_1, \ldots E_K$, from our training set.
- Now, **how can we use these centroids in the loss function of a neural network, in order to impose the quality of "natural clustering"?**

Centroid-Clustering Loss in Neural Networks

If the following two criteria hold, then the data will be easily clusterable (in the latent space):

- *Centroid-Attraction*: samples belonging to class C should be **close to the centroid** of class C.
- *Centroid-Repulsion*: samples NOT belonging to class C should be **far away from the centroid** of class C.

Centroid-Clustering Loss in Neural Networks

We can express these criteria with explicit loss functions that work over the latent space:

- *Centroid-Attraction*: **minimize** the distance between samples and the centroids of their classes.
- *Centroid-Repulsion*: **maximize** the distance between samples and the centroids of other classes.

Centroid-Clustering Loss: Measuring Distance

- How should we measure how “close” something is to something else?

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- If we are trying to maximize a distance, we probably need to use a distance function (measure of similarity) that does not diverge to infinity.

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- How should we measure how “close” something is to something else?
- If we are trying to maximize a distance, we probably need to use a distance function (measure of similarity) that does not diverge to infinity.
- So, no euclidean distance!

Centroid-Clustering Loss: Measuring Distance *with Cosine Distance*

- Let's use **cosine distance**!
    - Half of 1 minus the cosine similarity between the vectors (cosine similarity is in [-1, 1]).

$$cosd(u, v) = \frac{1}{2}\left(1 - \frac{u \cdot v}{||u||_2||v||_2}\right)$$

Centroid-Clustering Loss: Measuring Distance *with Cosine Distance*

- Let's use **cosine distance**!
  - If cosd(u,v)=0 then they are oriented in same direction.
  - If cosd(u,v)=1 then they are in opposite directions.

$$cosd(u, v) = \frac{1}{2}\left(1 - \frac{u \cdot v}{||u||_2||v||_2}\right)$$

Centroid-Clustering Loss: Measuring Distance *with Cosine Distance*

- Let's use **cosine distance**!
  - Computes the "angle between two vectors"
  - Magnitude invariant
  - Constrained between 0 and 1

Centroid-Clustering Loss: Measuring Distance *with Cosine Distance*

- Let's use **cosine distance**!
  - Computes the "angle between two vectors"
  - Magnitude invariant
  - Constrained between 0 and 1
  - Best understanding: **measures the squared euclidean distance between two vectors when projected onto the unit hypersphere.**

Centroid-Clustering Loss: Measuring Distance *with Cosine Distance*

- "But cosine-distance is less expressive since it is magnitude invariant!" *one might say...*

Centroid-Clustering Loss: Measuring Distance *with Cosine Distance*

- "But cosine-distance is less expressive since it is magnitude invariant!" *one might say…*
- It is well known that, in high dimensional spaces, euclidean distance is not meaningful and actually problematic due to hypersensitivity to small perturbations.
- So, this property of cosine-distance may actually be desirable, may make it *more expressive*! (Charu et al., 2001)
- But I'm open to suggestions for other distance metrics! Particularly ones that can be expressed in pure matrix form.

Centroid-Clustering Loss: Measuring Distance *with Cosine Distance*

- Note that, whatever distance function we choose, the model will learn non-linear transformations to manifest its properties as much as possible.
- So, perhaps, the distance function is not super decisive since the network will adapt to it regardless.

Centroid-Clustering Loss in Neural Networks

Centroid-Attraction: **minimize** the distance between samples and the centroids of their classes.

$$\mathbf{L}_{Att-SC} = \frac{\lambda_1}{n} \sum_{k=1}^{K} \sum_{i \in C_k} d(\boldsymbol{\mu}_k, \mathbf{h}_i)$$

Centroid-Repulsion: **maximize** the distance between samples and the centroids of other classes.

$$\mathbf{L}_{Rep-SC} = -\frac{\lambda_2}{n(K-1)} \sum_{k=1}^{K} \sum_{j \notin C_k} d(\boldsymbol{\mu}_k, \mathbf{h}_j)$$

Centroid-based Inference in Neural Networks

Note, if the *Centroid-Attraction* and *Centroid-Repulsion* criteria hold, and if the model has properly generalized, *then we **do not need an output layer** for our model.*

Centroid-based Inference in Neural Networks

Note, if the *Centroid-Attraction* and *Centroid-Repulsion* criteria hold, and if the model has properly generalized, *then we* ***do not need an output layer*** *for our model.*

Instead, we predict that the class of a new sample, *x*, is the class of the training-set centroid to which it is closest. E.g., `class(x) = argmin_c d(h(x), E_c)`

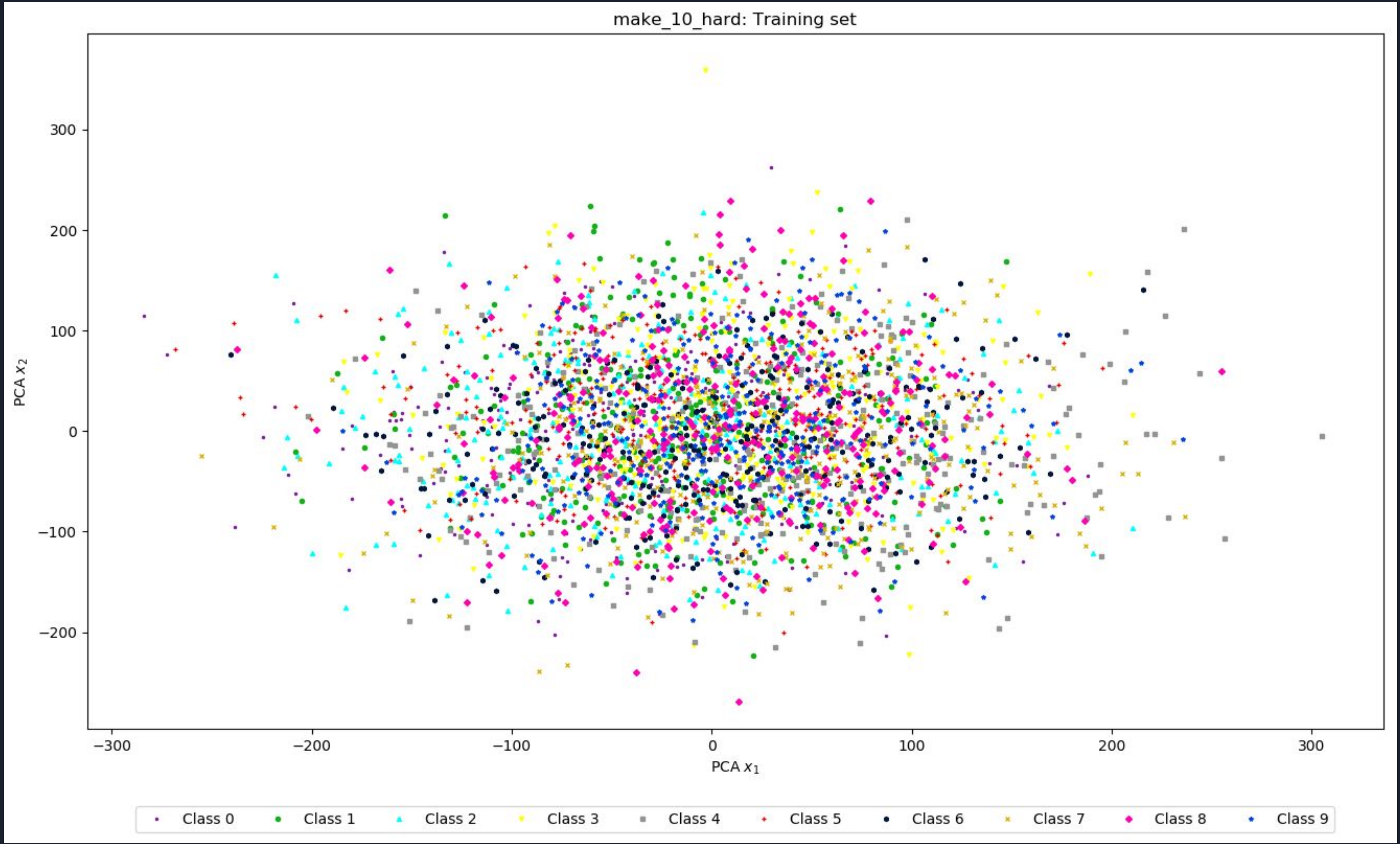
Summary of our Clustering-Oriented Representation Learning Network

- **No output layer**, works at the level of representation
- Dynamically maintains representations of the classes, the latent categorical centroids
- Uses clustering-oriented loss to optimize the network
    - **Attract** samples to their centroids
    - **Repulse** samples from other centroids
- Uses the centroids to perform inference

Experimental Design
(e.g., But does it work?)

We experiment with synthetic data to isolate model design from the specificities of working with real datasets.

- 3,400 training samples, 600 validation, 1000 test
- 1000 features per sample
- 10 classes


make_10_hard: Training set
PCA x_2
PCA x_1
300
200
100
0
−100
−200
−300
−200
−100
0
100
200
300
Class 0
Class 1
Class 2
Class 3
Class 4
Class 5
Class 6
Class 7
Class 8
Class 9

Dataset

Very hard! Very much *not* linearly separable!

Lots of noise!

Logistic regression only gets 20% accuracy!

SVM with RBF kernel (with highly tuned C) only gets 63% accuracy!

Experiments

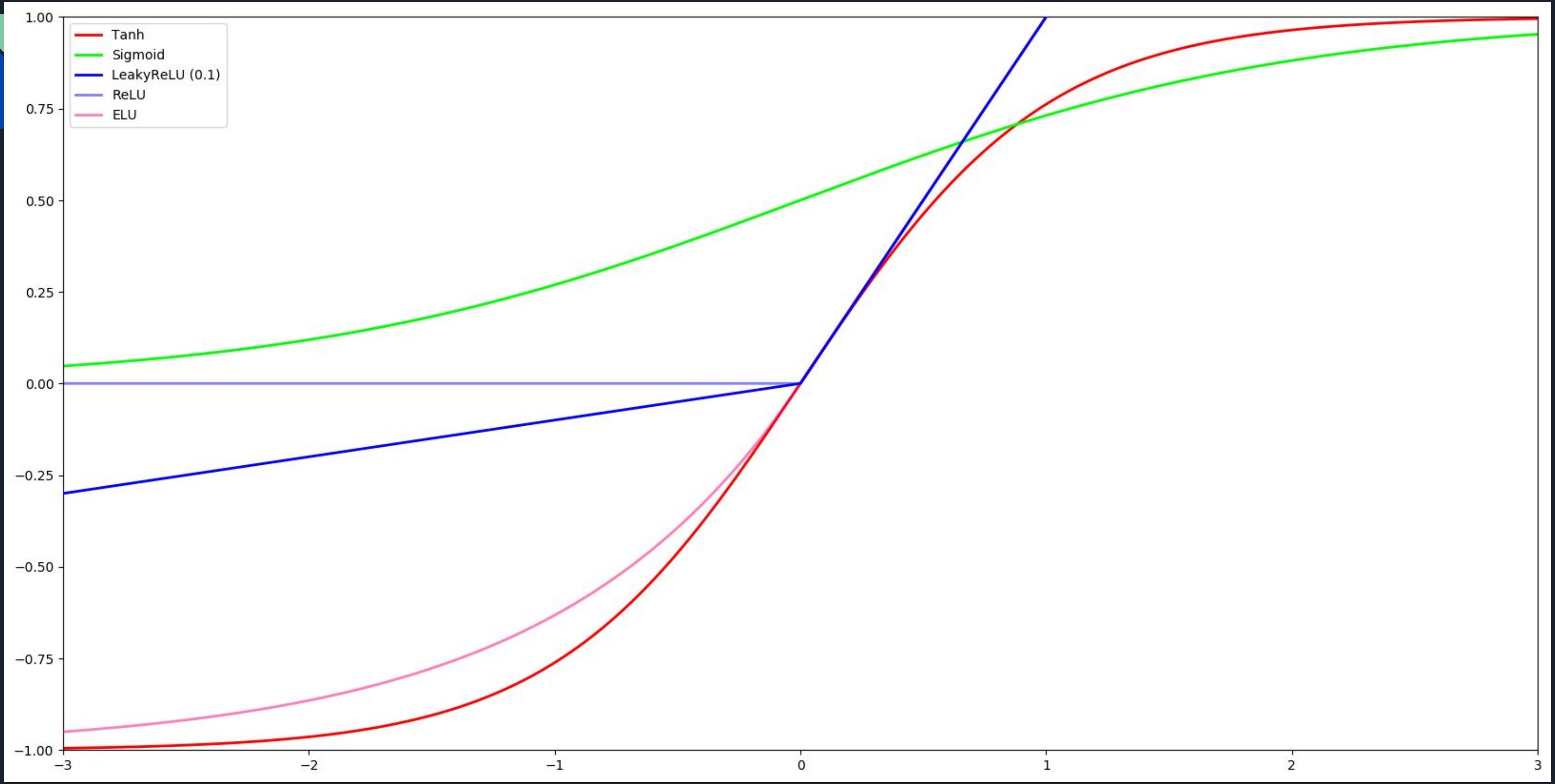
If our Centroid-Clustering loss is good, then the model trained with it should:

- Be better than other models
- Really should be better than a CCE feed-forward neural network

Parameter Tuning

Tested several thousand different neural network architecture variants for our model, including:

- Activation functions (Tanh, ReLU, LeakyReLU, PreLU…)
- Batch size (100, 340, 1700, 3400)
- Learning rate (many)
- Number and dimensionality of hidden layers (very many)



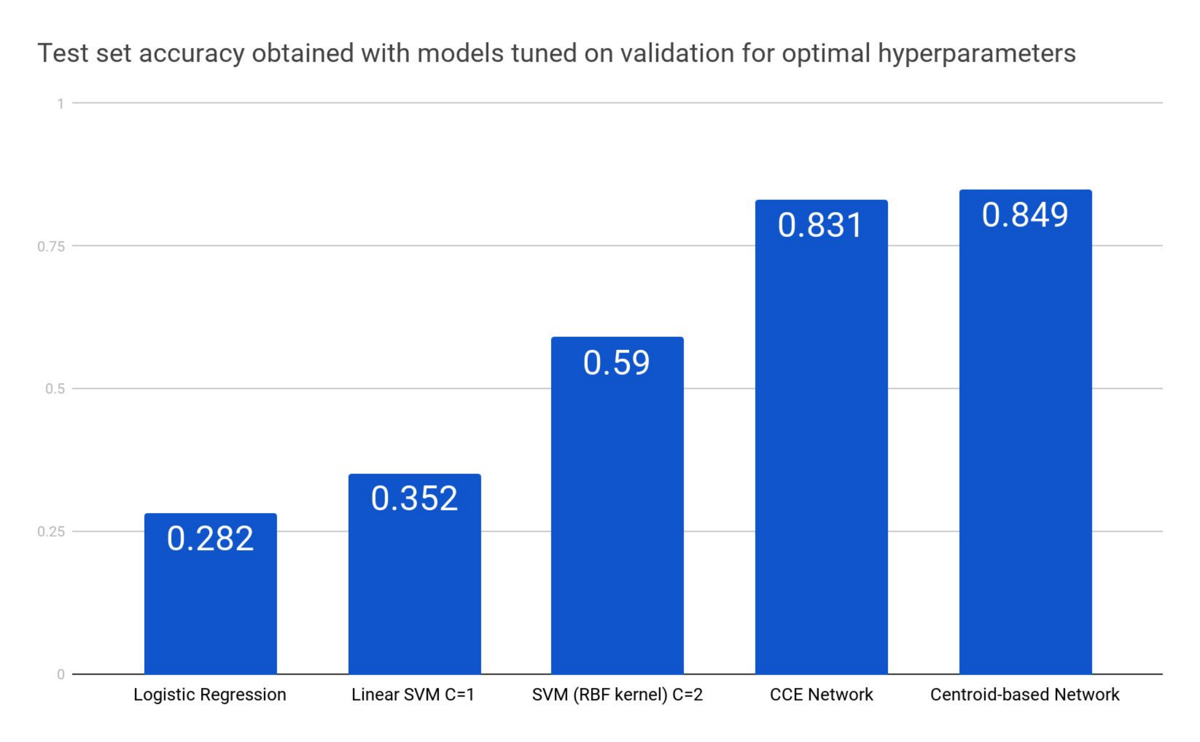
Tanh
Sigmoid
LeakyReLU (0.1)
ReLU
ELU
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
−3
−2
−1
0
1
2
3

Parameter Tuning - Results

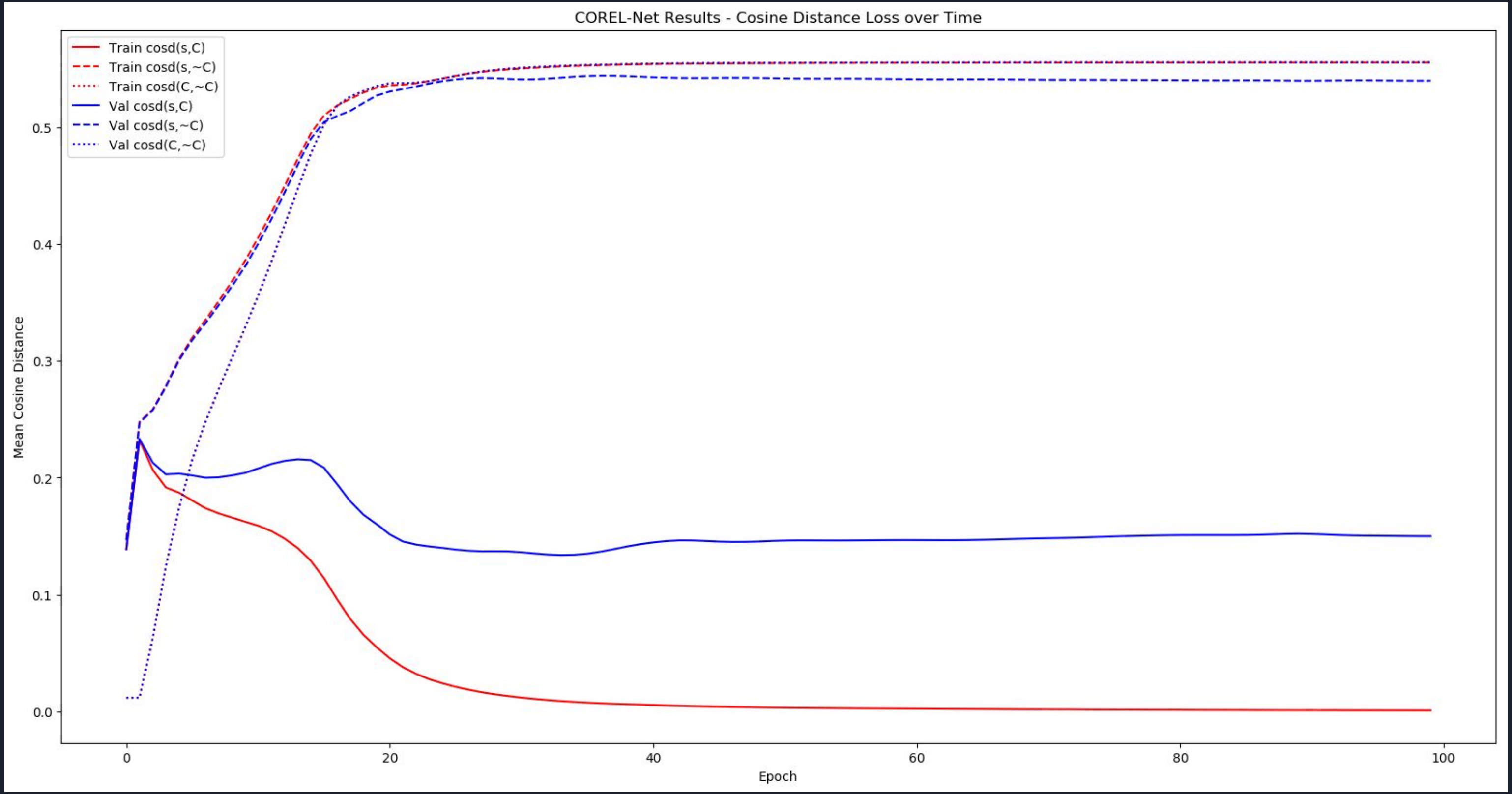
For our Centroid-based network, we found the following parameter settings were very important for obtaining optimal validation set accuracy:

- Using LeakyReLU, not ReLU (and definitely not Tanh!)
- Testing different variants of bottleneck networks, 3 layers worked quite well
  - E.g., Layer sizes [1000 -> 2048 -> 128 -> 4096]

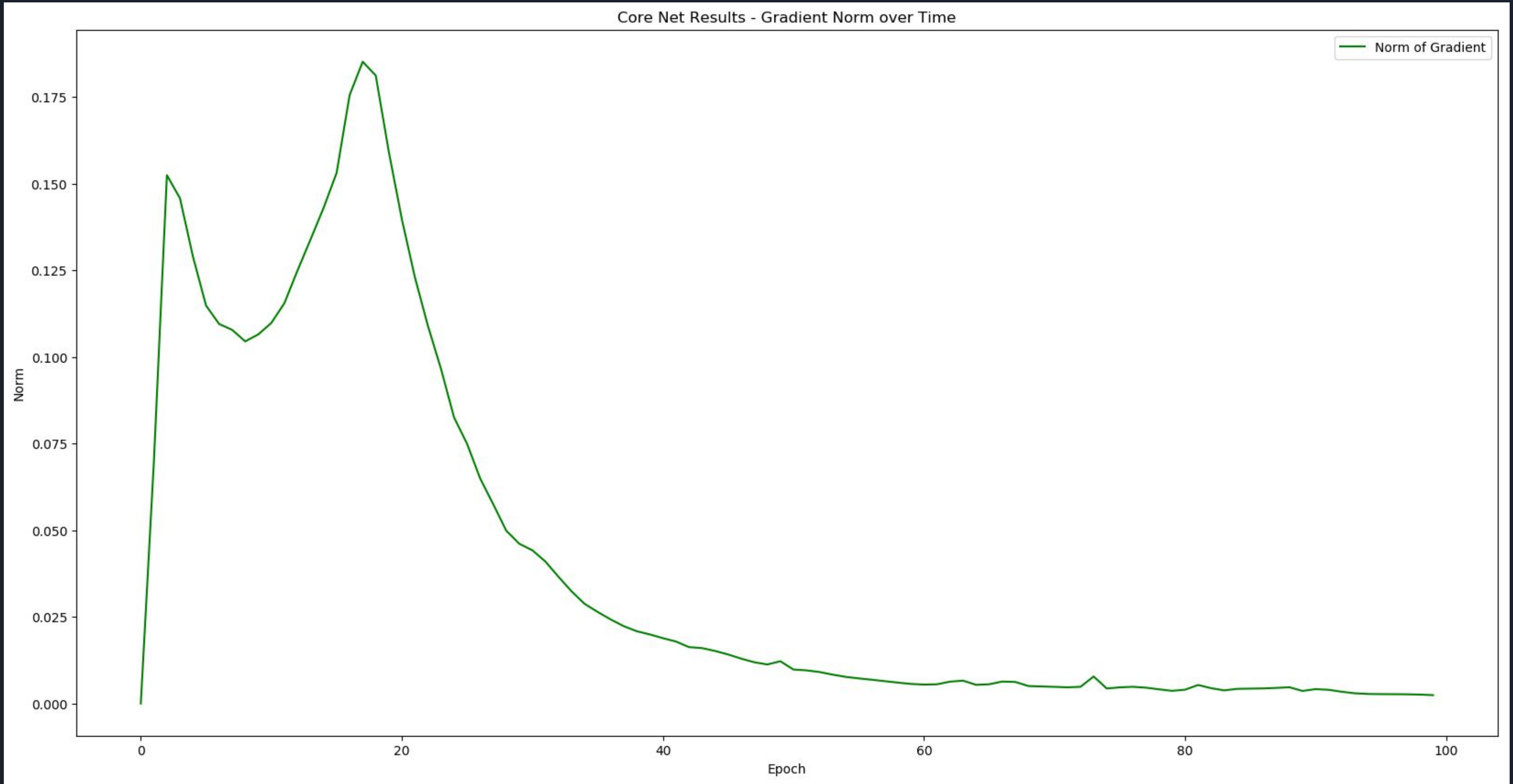
Final Test Set Results



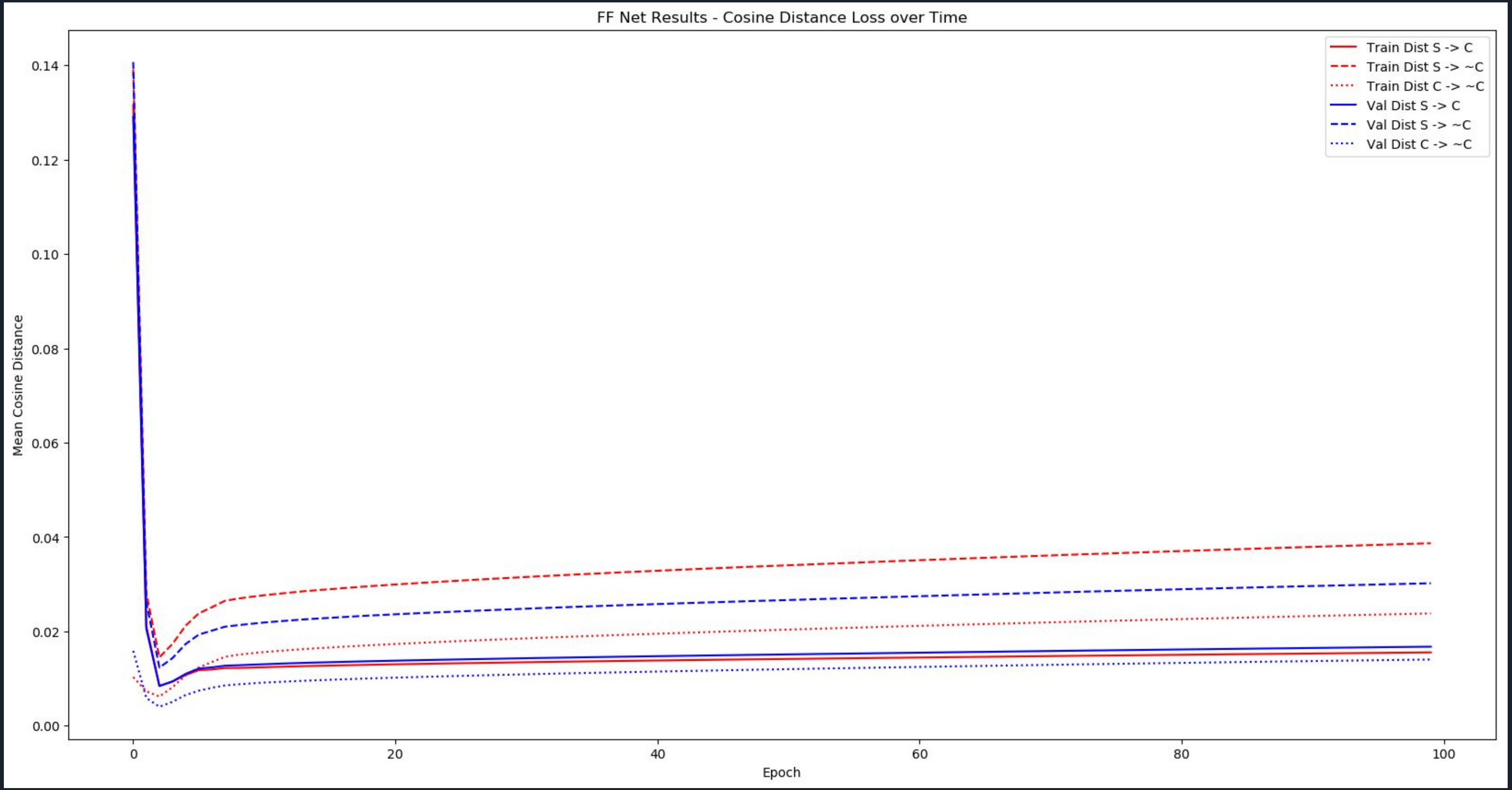
Learning to Cluster - Centroid Net



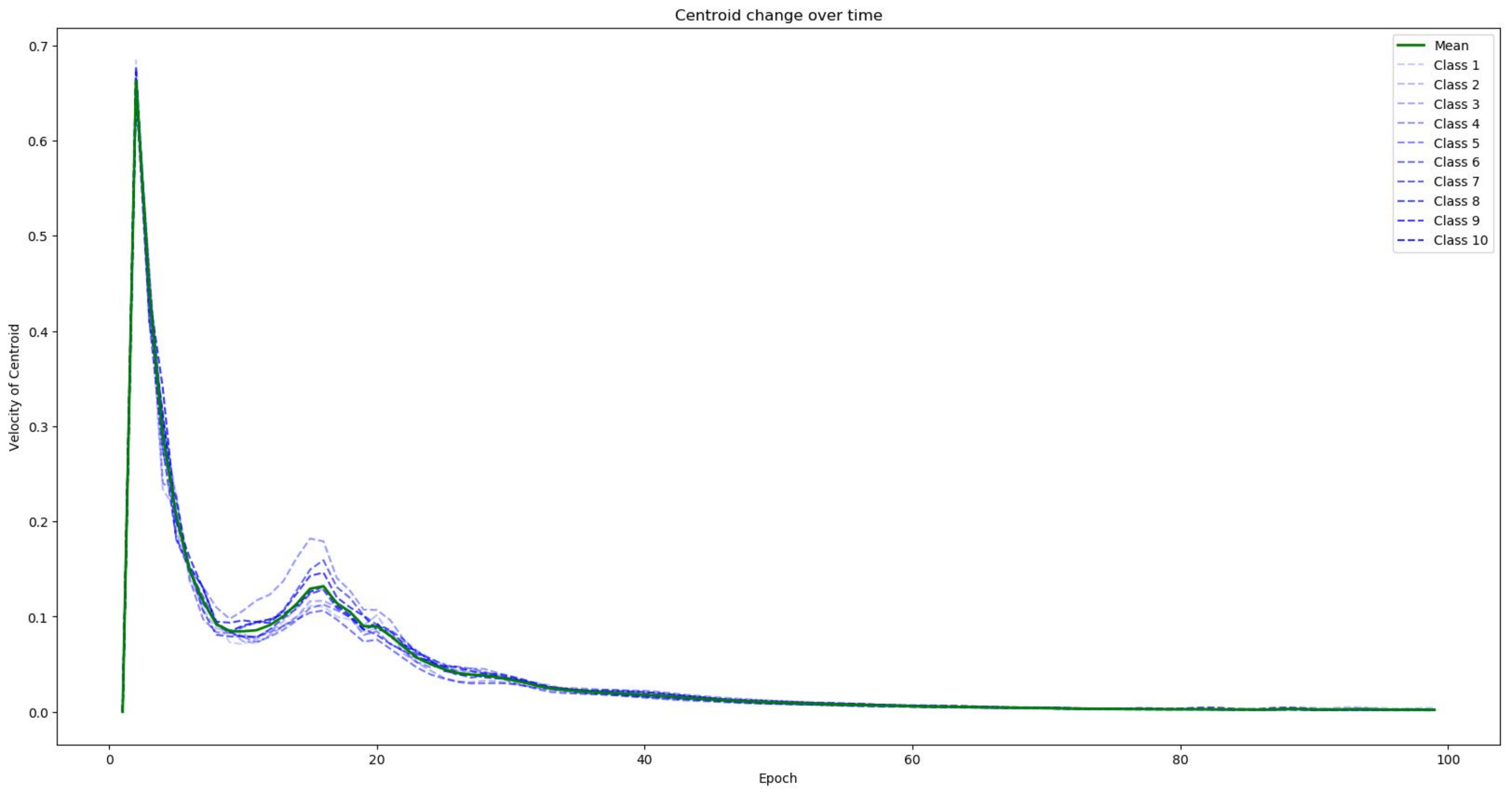
Norm of Gradient Over Time - Centroid Net



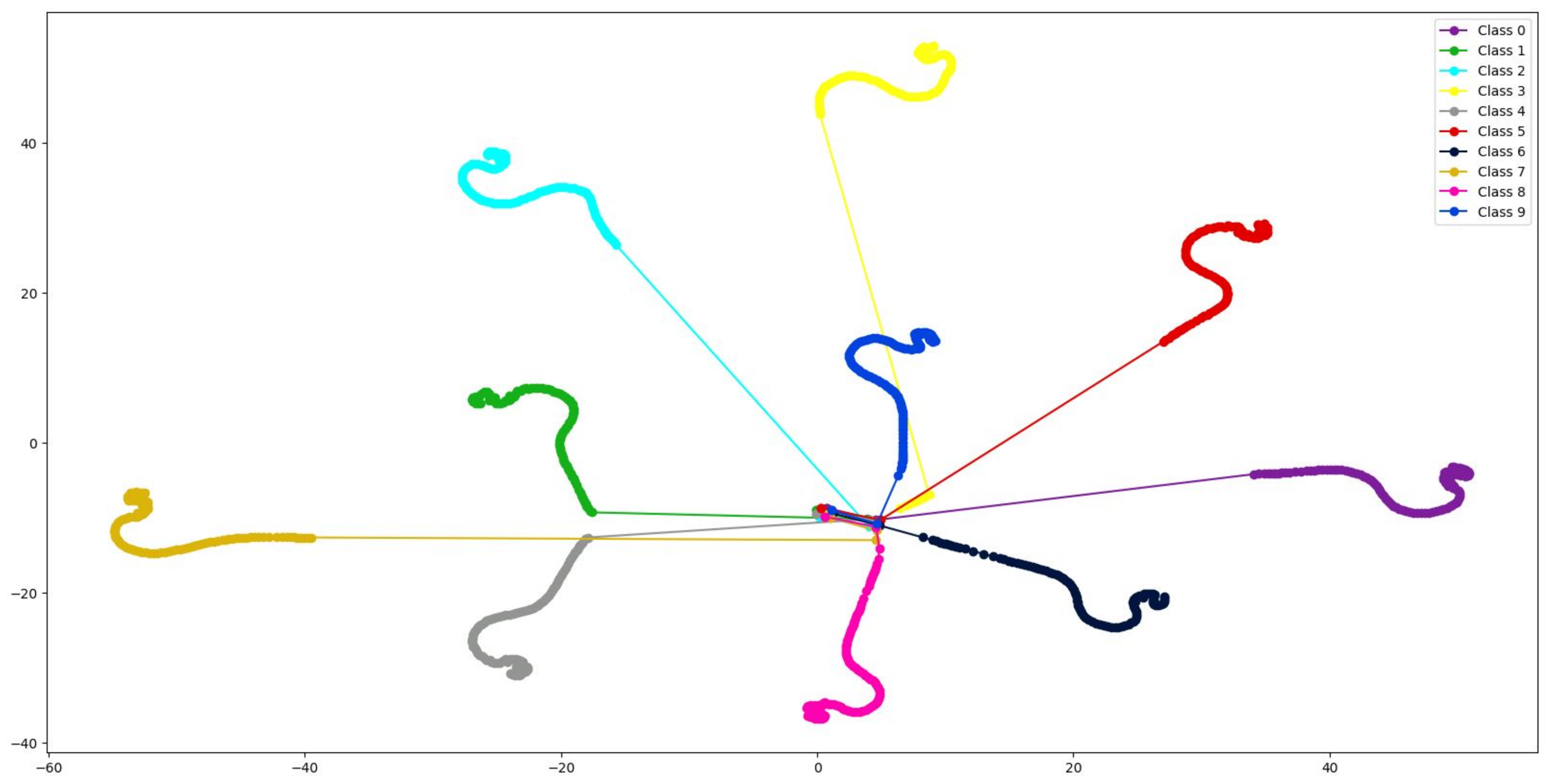
Learning to Cluster - CCE Net



Centroid Changes - Centroid Net



Centroid Changes during Training



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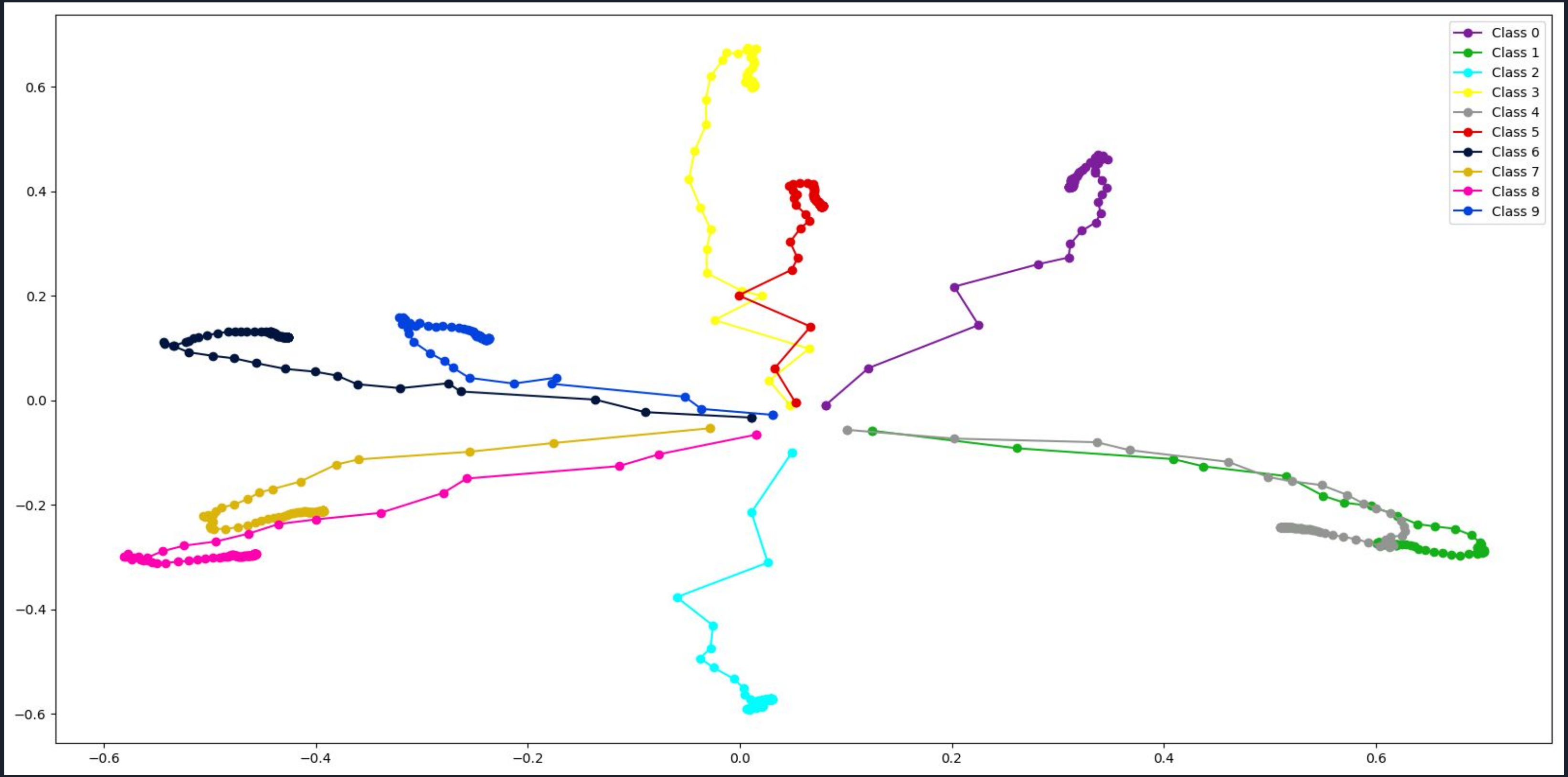
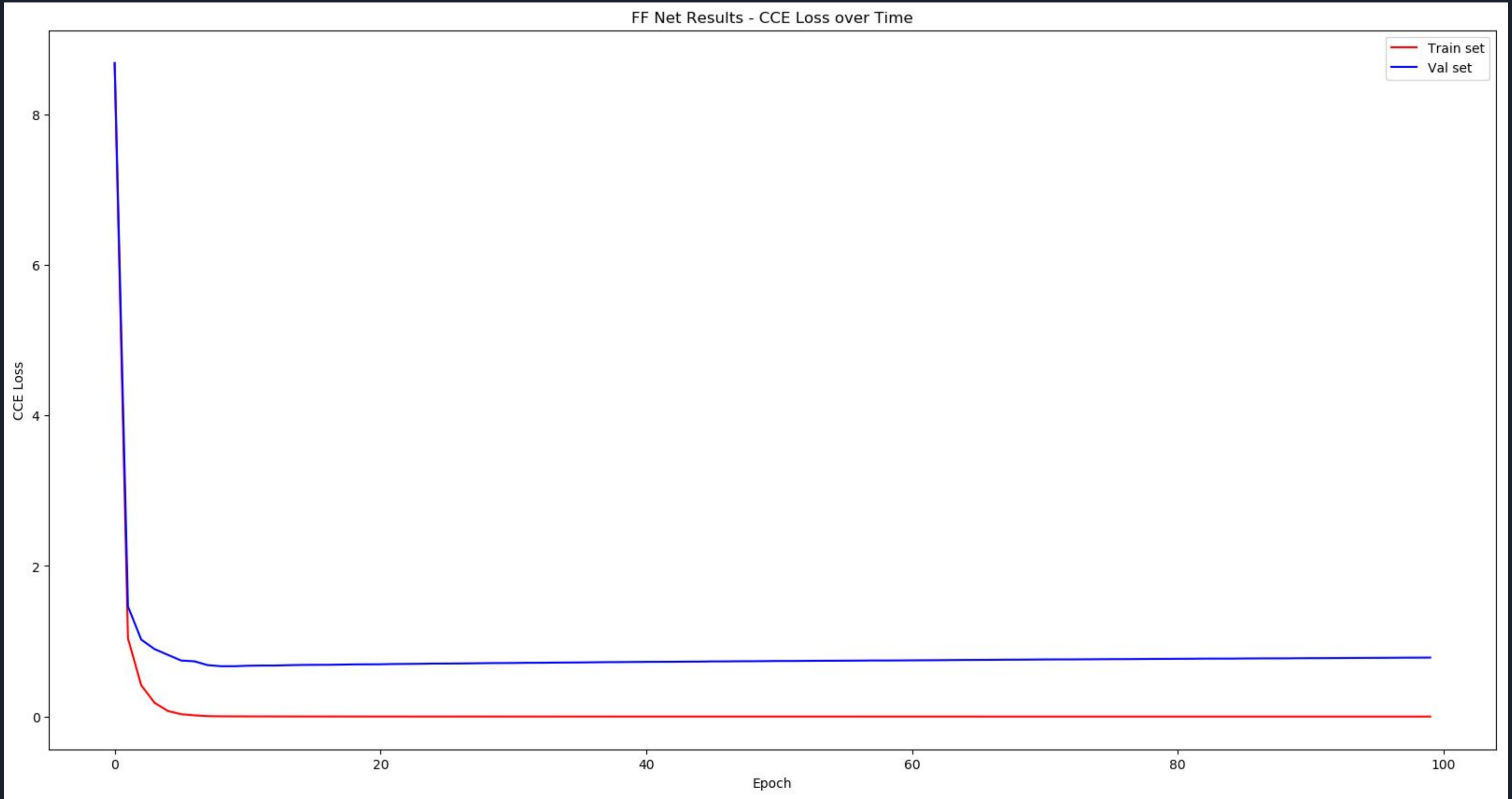


Learning to Predict - CCE Network



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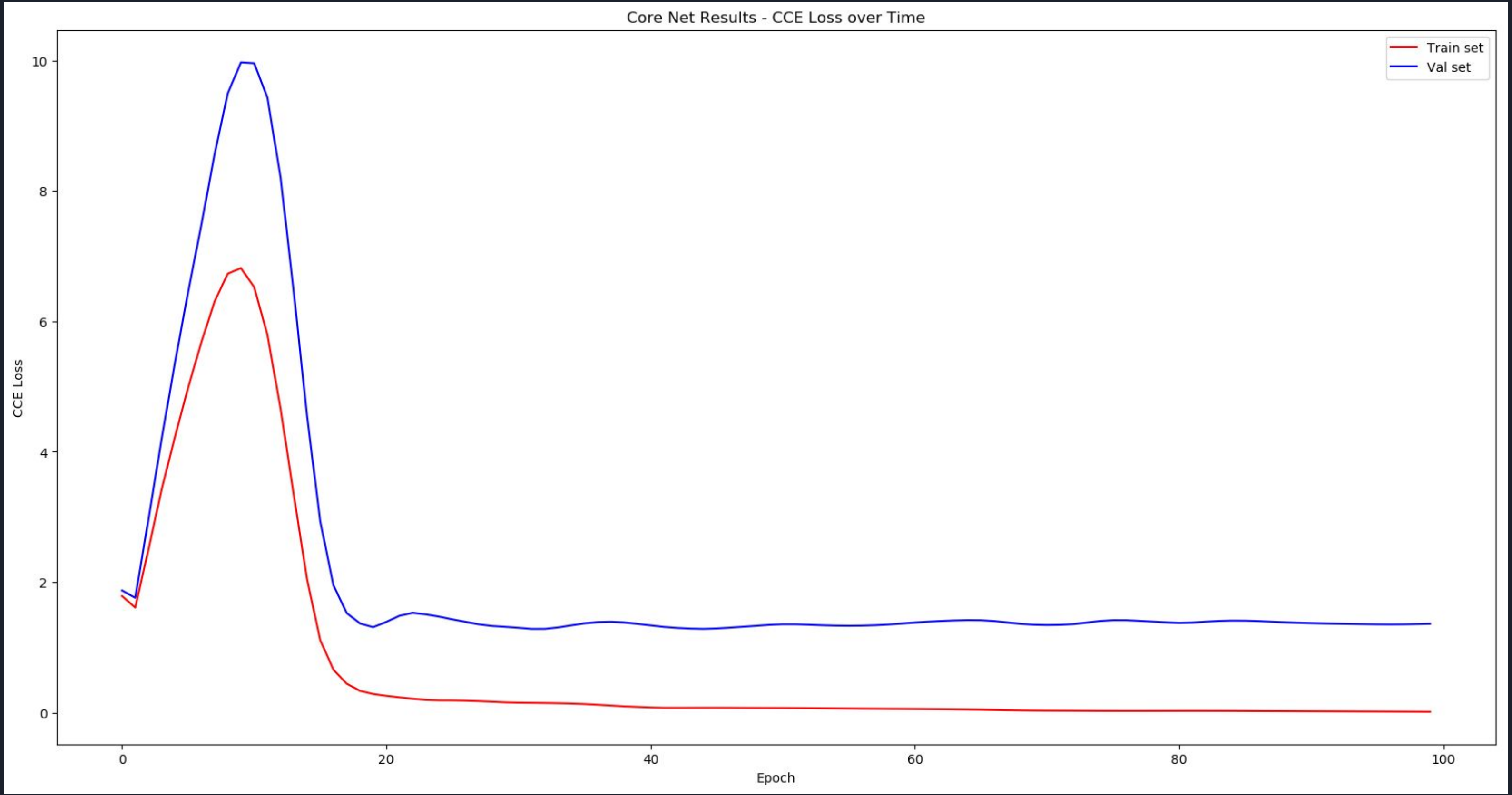
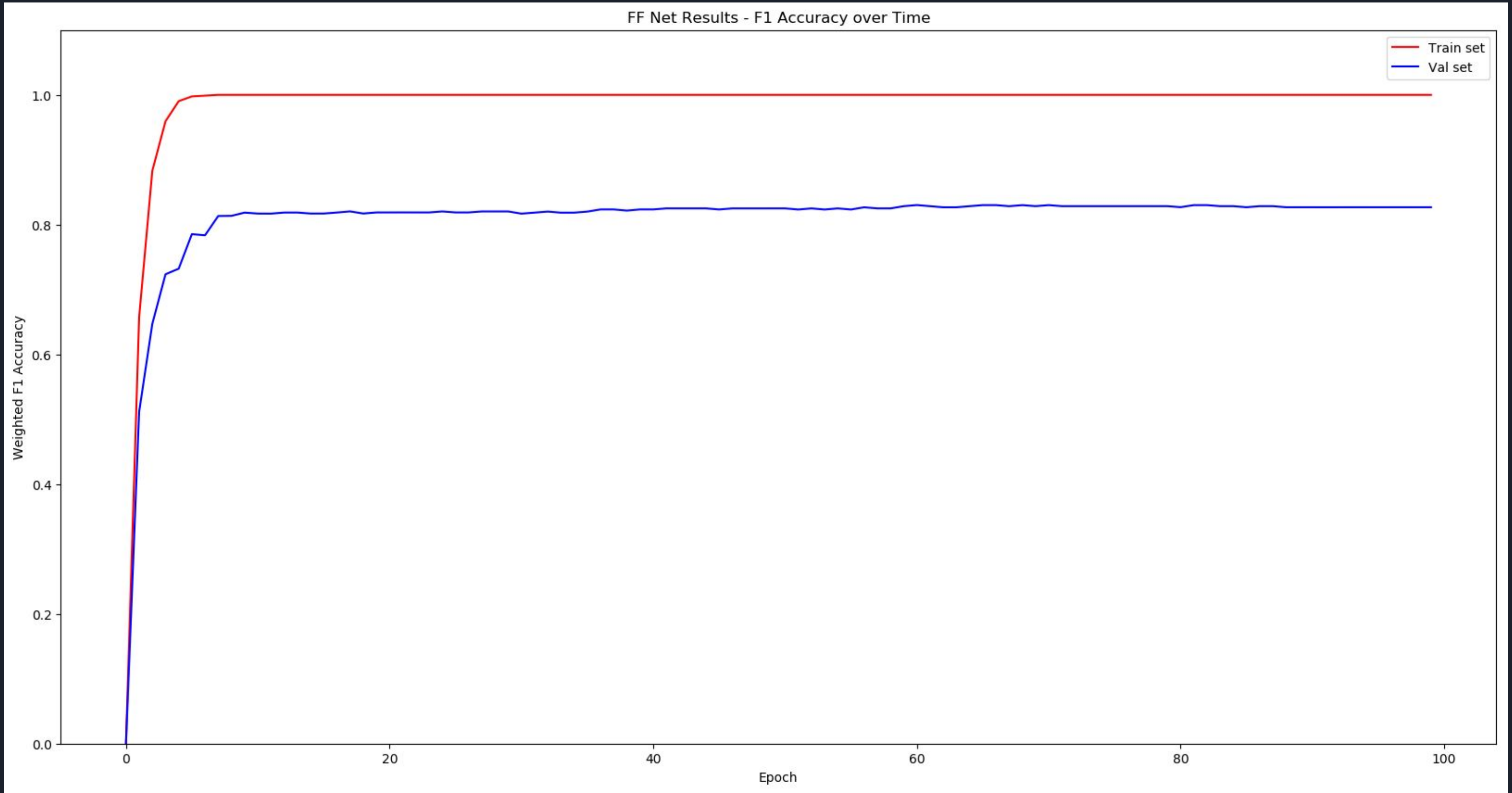


Accuracy Over Time - CCE Network



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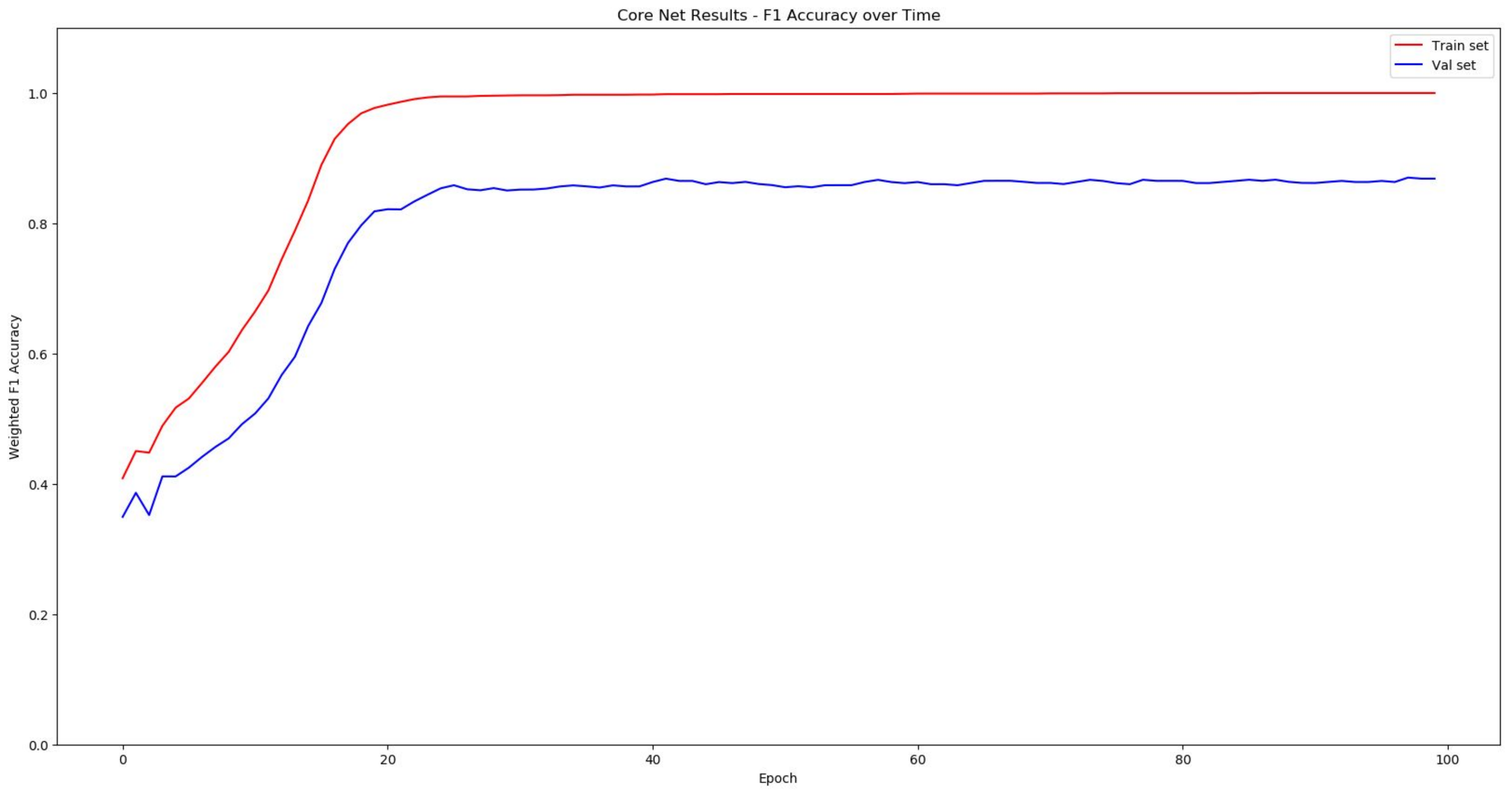
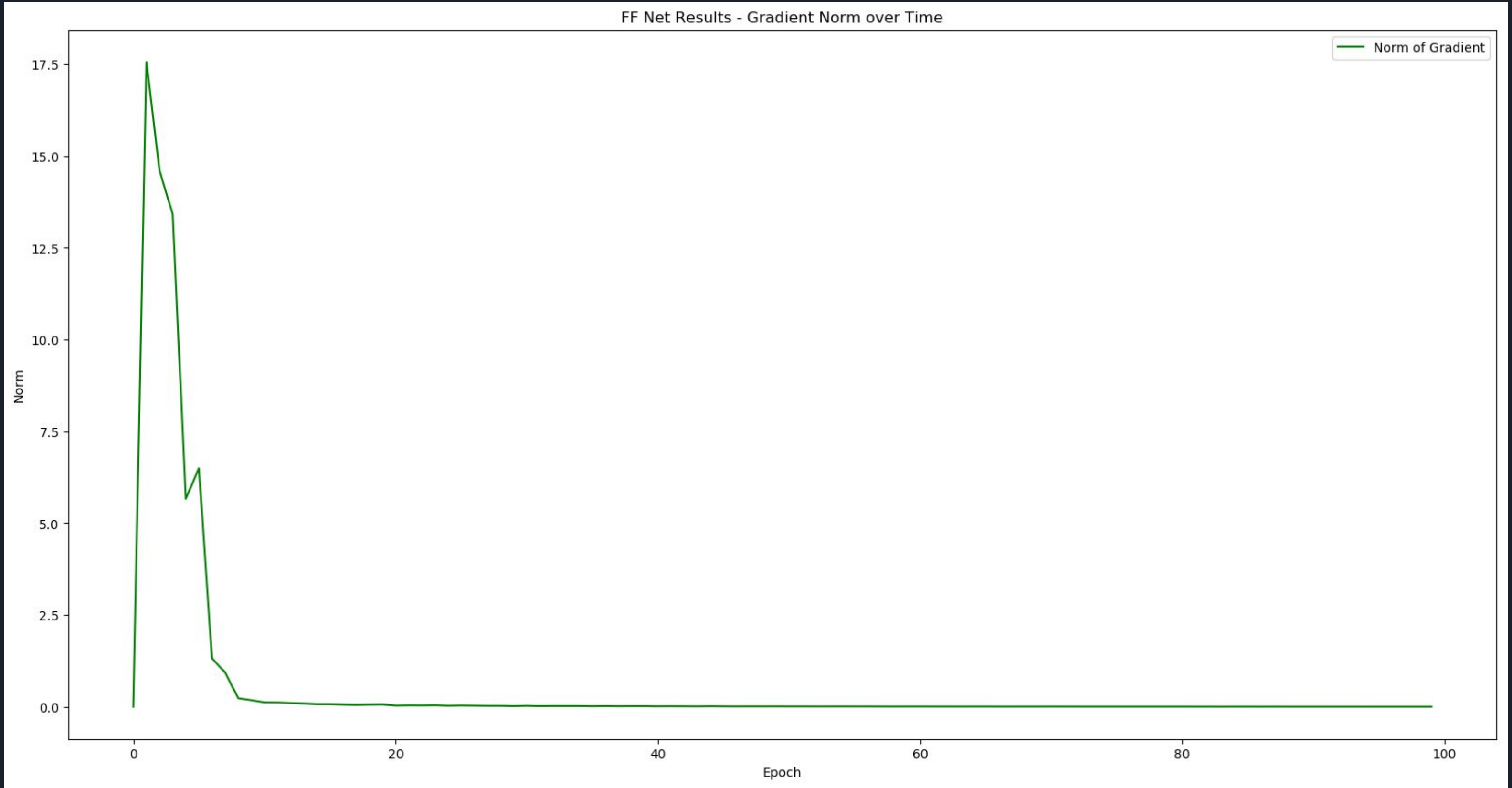
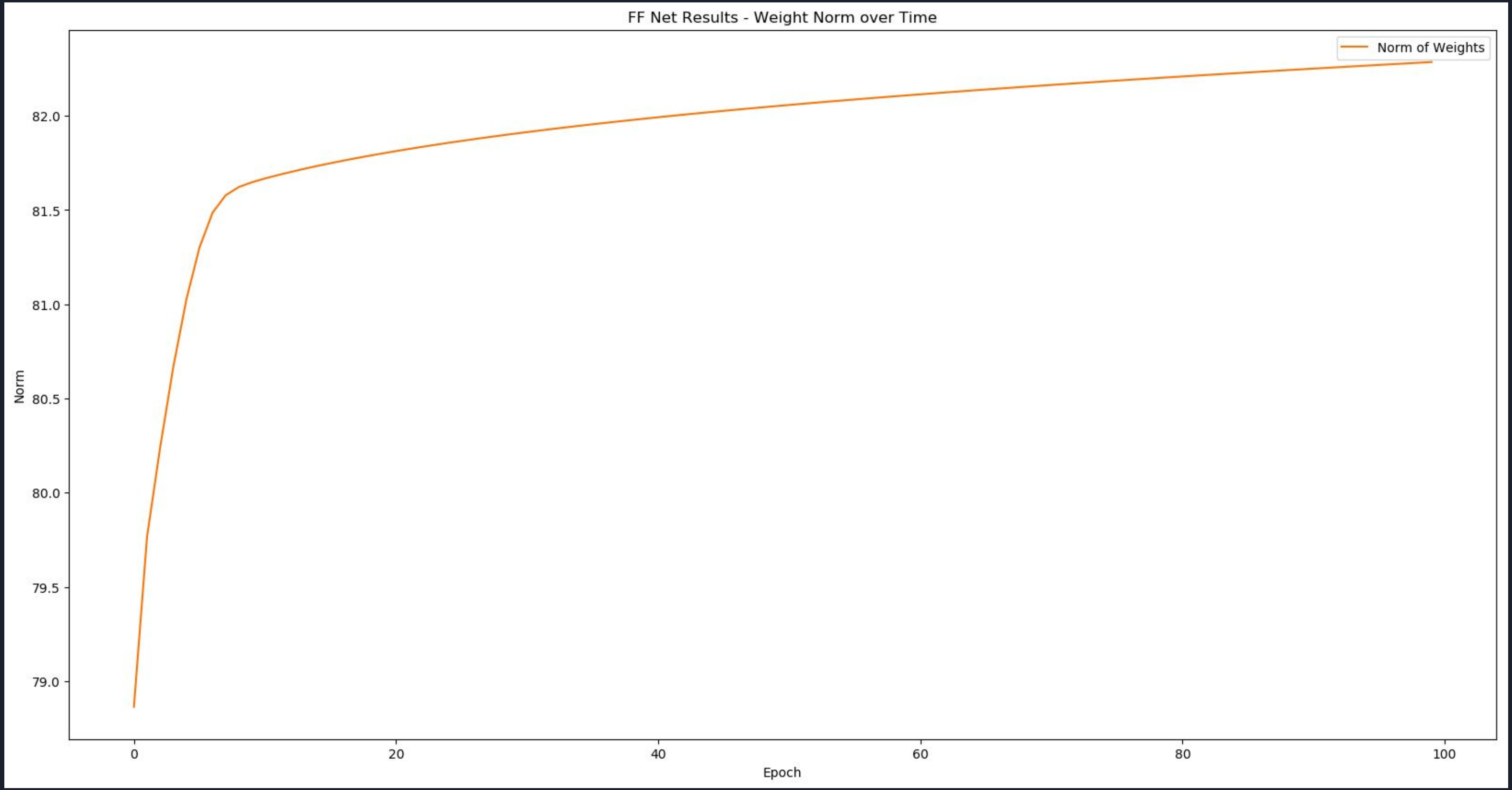


Norm of Gradient Over Time - CCE Net



Norm of Weights Over Time - CCE Net



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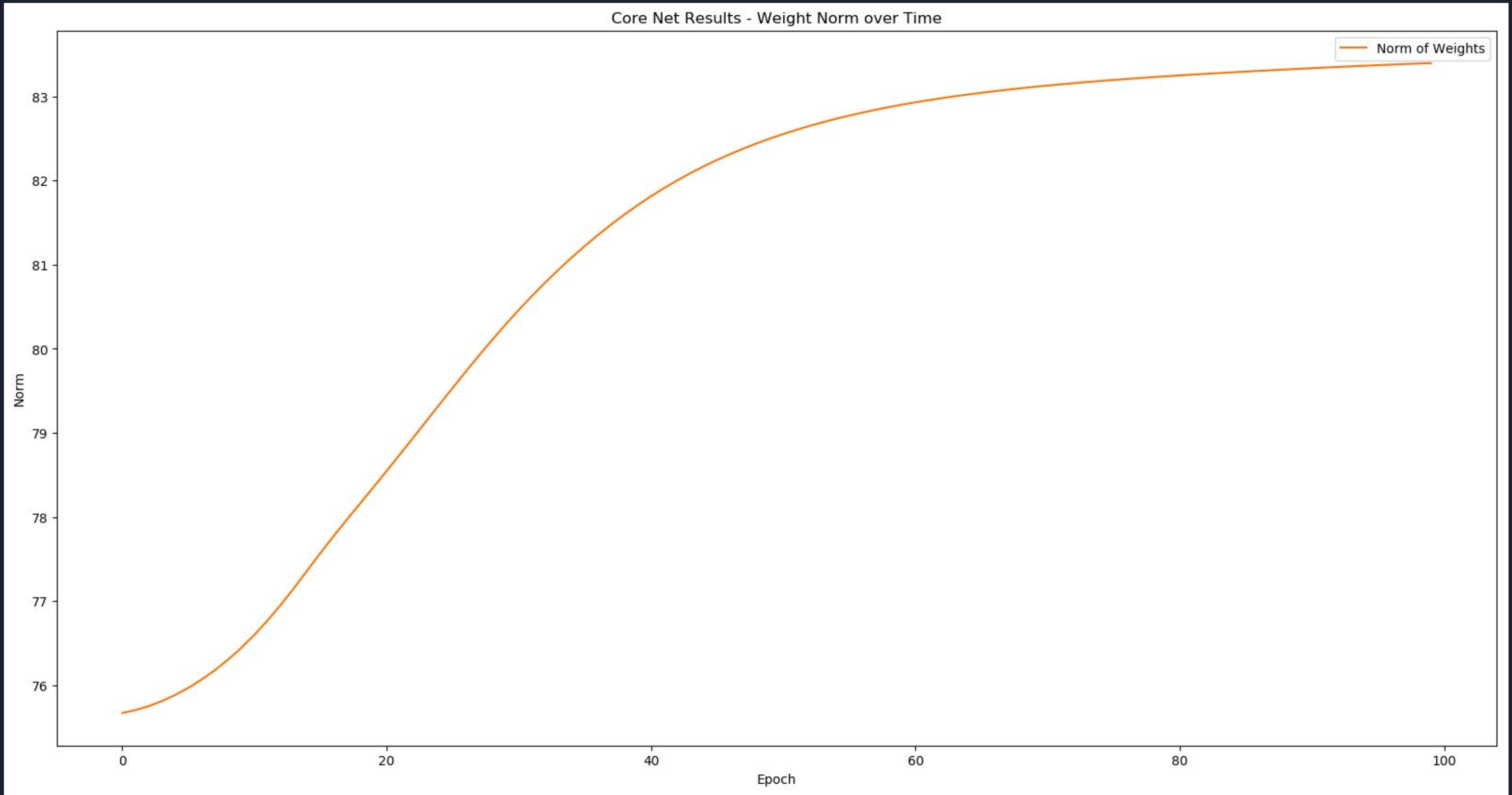
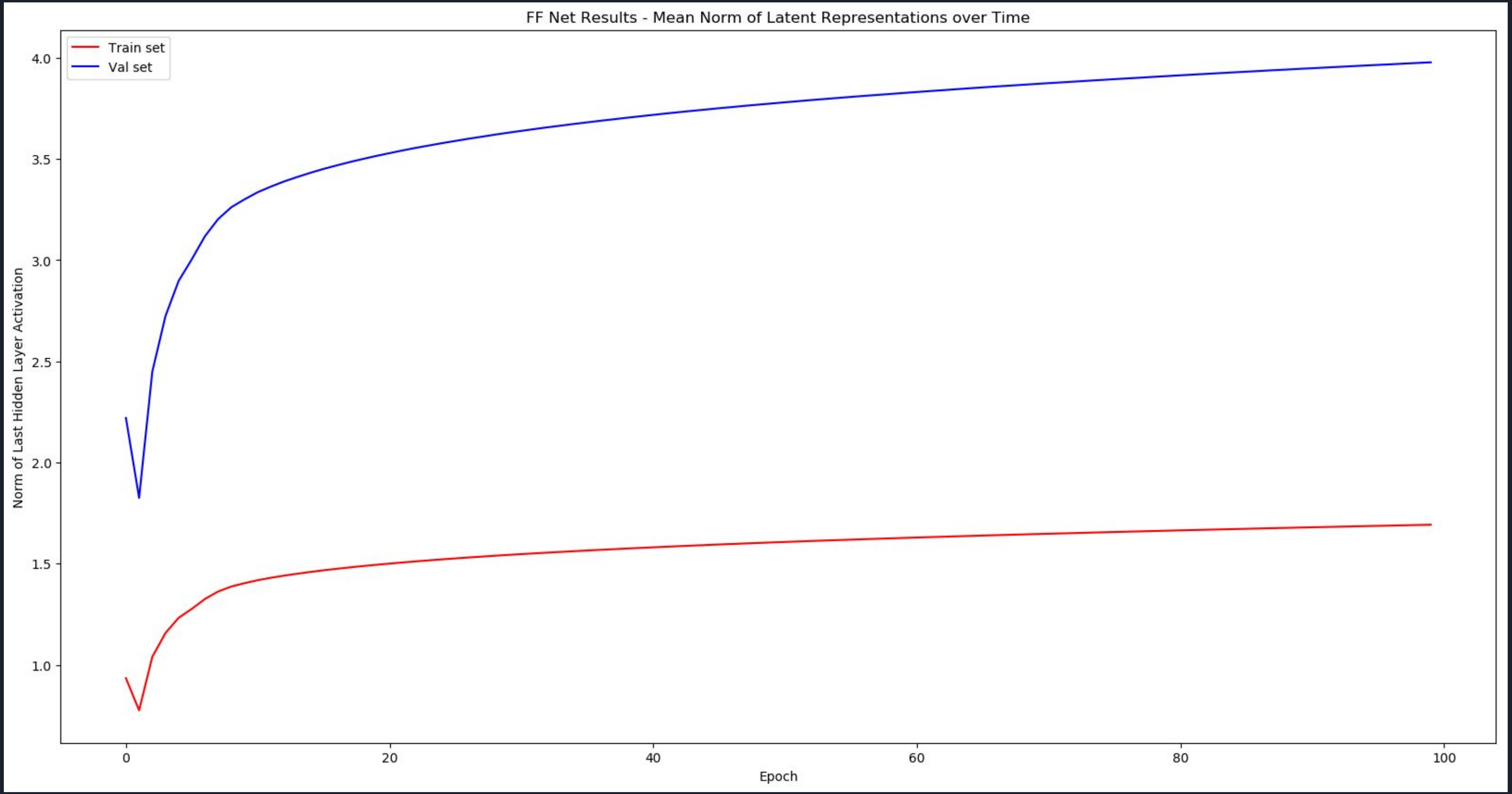


Norm of Reps. over time - CCE Net



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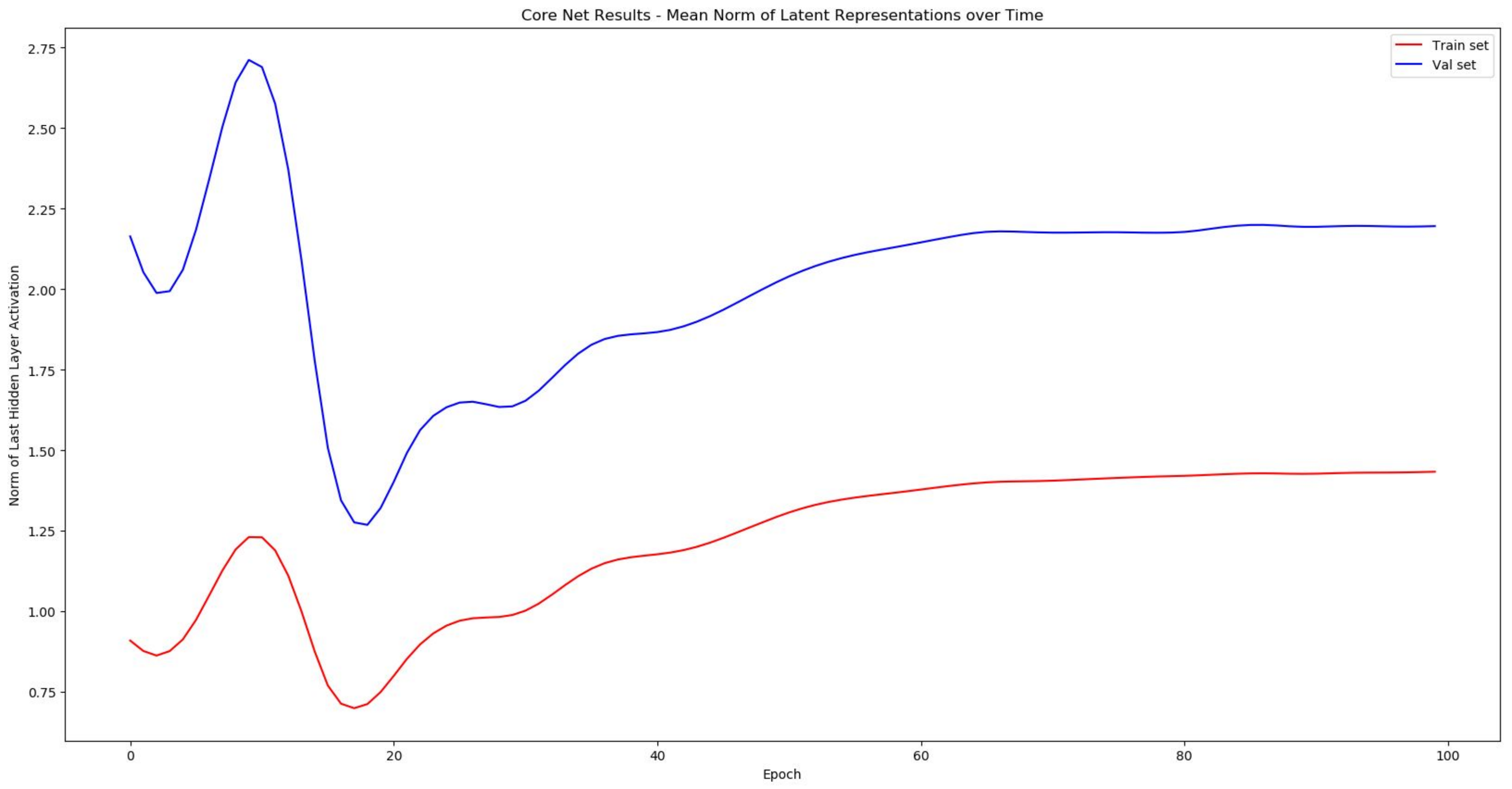

References

(Bengio *et al.*, 2013) - Bengio, Yoshua, Aaron Courville, and Pascal Vincent. "Representation learning: A review and new perspectives." IEEE transactions on pattern analysis and machine intelligence 35.8 (2013): 1798-1828.

(Charu et al., 2001) - Charu C Aggarwal, Alexander Hinneburg, and Daniel A Keim. “On the surprising behavior of distance metrics in high dimensional spaces”. In: ICDT. Vol. 1. Springer. 2001, pp. 420–434.

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- Was it by:
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  - Not writing classes?
  - Handwriting the results of experiments on some scrap paper?

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- **Surprise:** I did the exact opposite of those things!
- My philosophy when doing research is:
  - **Why not be more lazy?**

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- **Surprise:** I did the exact opposite of those things!
- My philosophy when doing research is:
  - **Why not be more lazy?**
  - Programmers are lazy - if you want to do less work and have an easier life, **write generalized code**!

neural_core_tests4.tsv

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kiank

Comments

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fx difficulty

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	difficulty	num_classes	make_blobs	MODEL_NAME	lr	activation	dense_layers	core	bsz	epochs	train_acc	val_acc	test_acc
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15	hard	10	FALSE	0.0005_LeakyReLU (0.1)_2048-256-4096_lam1_1-lam2_1-lam3_0_3400_100	0.0005	<function <la	[2048, 256, 4096]	{'lam1': 1, 'lam2': 1, 'lam3': 0}	3400	100	0.9982356956	0.8683563003	0.8431521768
16	hard	10	FALSE	0.00065_LeakyReLU (0.1)_2048-256-4096_lam1_1-lam2_1-lam3_0_1700_100	0.00065	<function <la	[2048, 256, 4096]	{'lam1': 1, 'lam2': 1, 'lam3': 0}	1700	100	0.9967651064	0.8680968406	0.8316953757
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18	hard	10	FALSE	0.0005_LeakyReLU (0.05)_2048-128-4096_lam1_1-lam2_1-lam3_0_1700_100	0.0005	<function <la	[2048, 128, 4096]	{'lam1': 1, 'lam2': 1, 'lam3': 0}	1700	100	0.9944111081	0.8671277098	0.842241404
19	hard	10	FALSE	0.00075_LeakyReLU (0.05)_2048-128-2048_lam1_1-lam2_1-lam3_0_3400_100	0.00075	<function <la	[2048, 128, 2048]	{'lam1': 1, 'lam2': 1, 'lam3': 0}	3400	100	0.9958823187	0.8667582456	0.8301301759
20	hard	10	FALSE	0.00065_LeakyReLU (0.1)_2048-128-1024_lam1_1-lam2_1-lam3_0_1700_100	0.00065	<function <la	[2048, 128, 1024]	{'lam1': 1, 'lam2': 1, 'lam3': 0}	1700	100	0.9958818889	0.8665009634	0.8480816049
21	hard	10	FALSE	0.0005_LeakyReLU (0.1)_2048-128-2048_lam1_1-lam2_1-lam3_0_1700_100	0.0005	<function <la	[2048, 128, 2048]	{'lam1': 1, 'lam2': 1, 'lam3': 0}	1700	100	0.9973529137	0.8652520914	0.8428763353
22	hard	10	FALSE	0.00075_LeakyReLU (0.005)_2048-256-4096_lam1_1-lam2_1-lam3_0_3400_100	0.00075	<function <la	[2048, 256, 4096]	{'lam1': 1, 'lam2': 1, 'lam3': 0}	3400	100	0.9985294132	0.8651721758	0.8384392187
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24	hard	10	FALSE	0.0005_LeakyReLU (0.1)_2048-256-512_lam1_1-lam2_1-lam3_0_1700_100	0.0005	<function <la	[2048, 256, 512]	{'lam1': 1, 'lam2': 1, 'lam3': 0}	1700	100	0.9985298294	0.8648541341	0.8239931993
25	hard	10	FALSE	0.00075_LeakyReLU (0.05)_2048-256-1024_lam1_1-lam2_1-lam3_0_3400_100	0.00075	<function <la	[2048, 256, 1024]	{'lam1': 1, 'lam2': 1, 'lam3': 0}	3400	100	0.9976470369	0.8648487248	0.8240430764
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27	hard	10	FALSE	0.00075_LeakyReLU (0.05)_2048-256-4096_lam1_1-lam2_1-lam3_0_3400_100	0.00075	<function <la	[2048, 256, 4096]	{'lam1': 1, 'lam2': 1, 'lam3': 0}	3400	100	0.9961759584	0.8648023673	0.8419349548
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29	hard	10	FALSE	0.00075_LeakyReLU (0.1)_2048-128-4096_lam1_1-lam2_1-lam3_0_3400_100	0.00075	<function <la	[2048, 128, 4096]	{'lam1': 1, 'lam2': 1, 'lam3': 0}	3400	100	0.9976474567	0.8636973242	0.8449513636
30	hard	10	FALSE	0.00065_LeakyReLU (0.1)_2048-128-4096_lam1_1-lam2_1-lam3_0_1700_100	0.00065	<function <la	[2048, 128, 4096]	{'lam1': 1, 'lam2': 1, 'lam3': 0}	1700	100	0.9997058932	0.8635035823	0.8358569104
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fx difficulty

	difficulty	num_classes	make_blobs	lr	activation	dense_layers	core	bsz	epochs	MODEL_NAME	epoch	weight_norm	gradient_norm	activation_normt	activation_normv	cce_losstrain	cce_lossval	attractive_samp_	attracti
2	hard	10	FALSE	0.00065_LeakyR	0.00065	LeakyReLU (0.1)	[2048, 256, 4096	{'lam1': 1, 'lam2':	3400	100	0	75.6654892	No Grad...	0.9192941464	2.196246134	1.797406197	1.889685512	0.133137092	0.130
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14	hard	10	FALSE	0.00065_LeakyR	0.00065	LeakyReLU (0.1)	[2048, 256, 4096	{'lam1': 1, 'lam2':	3400	100	12	76.94435883	0.1211752727	1.165448142	2.463157349	4.897107601	8.181108475	0.1428721696	0.20
15	hard	10	FALSE	0.00065_LeakyR	0.00065	LeakyReLU (0.1)	[2048, 256, 4096	{'lam1': 1, 'lam2':	3400	100	13	77.14120483	0.1312593466	1.06344188	2.205767212	3.601153374	6.609869003	0.1340707839	0.201
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Java Update Available

Principles for Good Research Practices

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- Use multiple files and classes to separate tasks.
- Code it like you will use it in the future.
- Save your results every time you get them!

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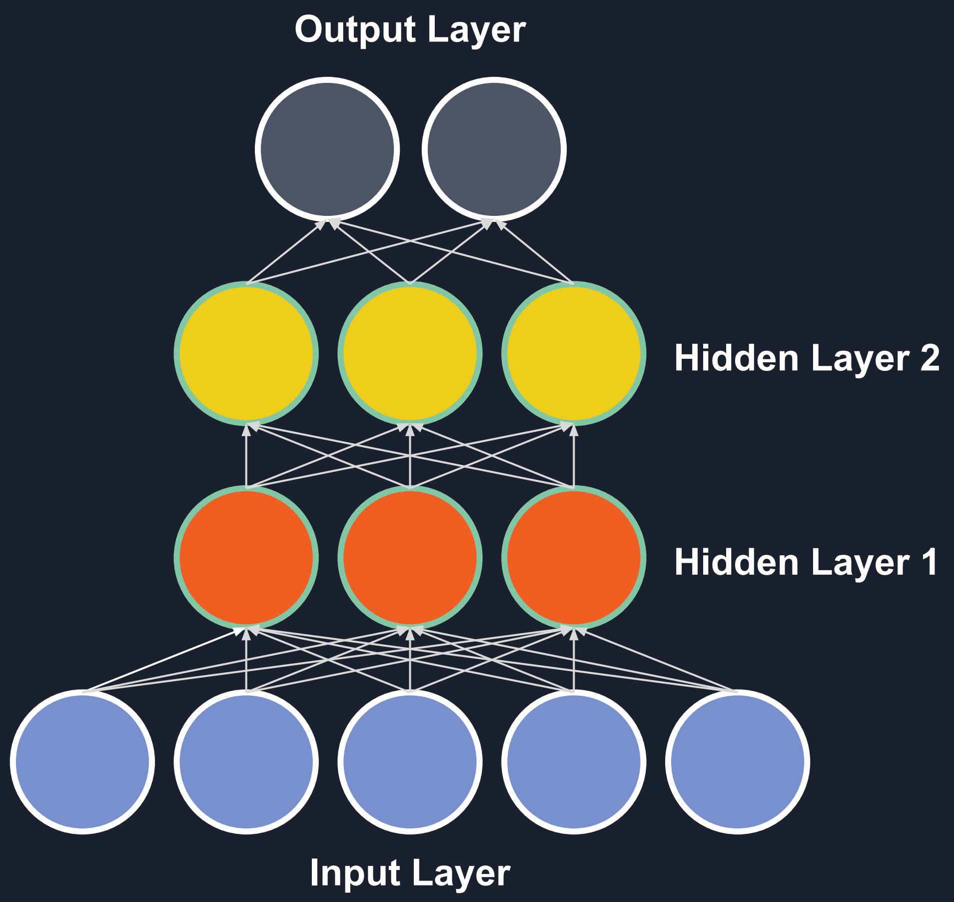
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Hidden Layer 2
Hidden Layer 1
Input Layer