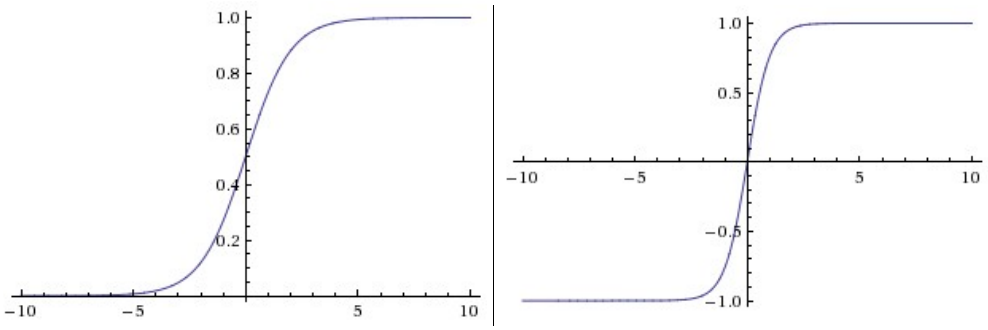
Lecture 5. Training neural networks I

Disclaimer: This note was modified from cs231n lecture notes by Prof. Li Fei-Fei at Stanford University.

Table of Contents:

Commonly used activation functions

Every activation function (or *non-linearity*) takes a single number and performs a certain fixed mathematical operation on it. There are several activation functions you may encounter in practice:



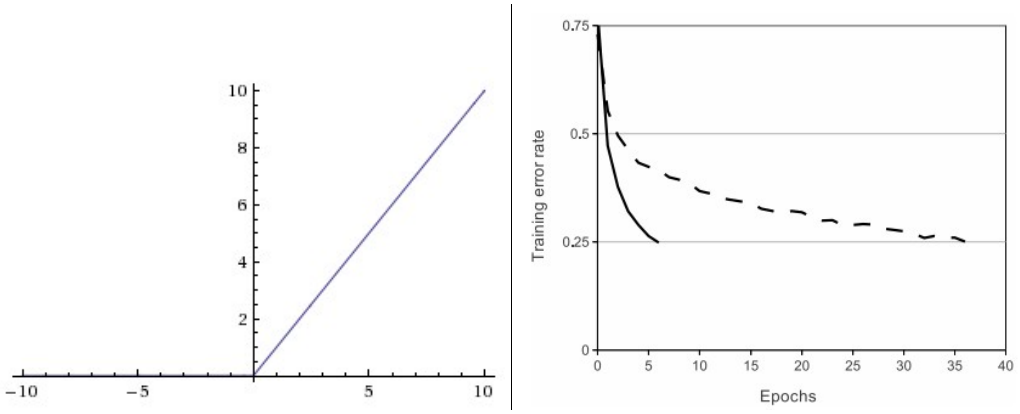
Left: Sigmoid non-linearity squashes real numbers to range between [0,1] **Right:** The tanh non-linearity squashes real numbers to range between [-1,1].

Sigmoid. The sigmoid non-linearity has the mathematical form $\sigma(x) = 1/(1+e^{-x})$ and is shown in the image above on the left. As alluded to in the previous section, it takes a real-valued number and "squashes" it into range between 0 and 1. In particular, large negative numbers become 0 and large positive numbers become 1. The sigmoid function has seen frequent use historically since it has a nice interpretation as the firing rate of a neuron: from not firing at all (0) to fully-saturated firing at an assumed maximum frequency (1). In practice, the sigmoid non-linearity has recently fallen out of favor and it is rarely ever used. It has two major drawbacks:

- *Sigmoids saturate and kill gradients*. A very undesirable property of the sigmoid neuron is that when the neuron's activation saturates at either tail of 0 or 1, the gradient at these regions is almost zero. Recall that during backpropagation, this (local) gradient will be multiplied to the gradient of this gate's output for the whole objective. Therefore, if the local gradient is very small, it will effectively "kill" the gradient and almost no signal will flow through the neuron to its weights and recursively to its data. Additionally, one must pay extra caution when initializing the weights of sigmoid neurons to prevent saturation. For example, if the initial weights are too large then most neurons would become saturated and the network will barely learn.
- *Sigmoid outputs are not zero-centered*. This is undesirable since neurons in later layers of processing in a Neural Network (more on this soon) would be receiving data that is not zero-centered. This has implications on the dynamics during gradient descent, because if the data coming into a neuron is always positive (e.g. $x > 0$ elementwise in $f = w^T x + b$)), then the gradient on the weights w will during backpropagation become either all be positive, or all negative (depending on the gradient of the whole expression f). This could introduce undesirable zig-zagging dynamics in the gradient updates for the weights. However, notice that once these gradients are added up across a batch of data the final update for the weights can have

variable signs, somewhat mitigating this issue. Therefore, this is an inconvenience but it has less severe consequences compared to the saturated activation problem above.

Tanh. The tanh non-linearity is shown on the image above on the right. It squashes a real-valued number to the range [-1, 1]. Like the sigmoid neuron, its activations saturate, but unlike the sigmoid neuron its output is zero-centered. Therefore, in practice the *tanh non-linearity is always preferred to the sigmoid nonlinearity.* Also note that the tanh neuron is simply a scaled sigmoid neuron, in particular the following holds: $\tanh(x) = 2\sigma(2x) - 1$.



Left: Rectified Linear Unit (ReLU) activation function, which is zero when x < 0 and then linear with slope 1 when x > 0. **Right:** A plot from Krizhevsky et al. (pdf) paper indicating the 6x improvement in convergence with the ReLU unit compared to the tanh unit.

ReLU. The Rectified Linear Unit has become very popular in the last few years. It computes the function $f(x) = \max(0, x)$. In other words, the activation is simply thresholded at zero (see image above on the left). There are several pros and cons to using the ReLUs:

- (+) It was found to greatly accelerate (e.g. a factor of 6 in Krizhevsky et al.) the convergence of stochastic gradient descent compared to the sigmoid/tanh functions. It is argued that this is due to its linear, non-saturating form.
- (+) Compared to tanh/sigmoid neurons that involve expensive operations (exponentials, etc.), the ReLU can be implemented by simply thresholding a matrix of activations at zero.
- (-) Unfortunately, ReLU units can be fragile during training and can "die". For example, a large gradient flowing through a ReLU neuron could cause the weights to update in such a way that the neuron will never activate on any datapoint again. If this happens, then the gradient flowing through the unit will forever be zero from that point on. That is, the ReLU units can irreversibly die during training since they can get knocked off the data manifold. For example, you may find that as much as 40% of your network can be "dead" (i.e. neurons that never activate across the entire training dataset) if the learning rate is set too high. With a proper setting of the learning rate this is less frequently an issue.

Leaky ReLU. Leaky ReLUs are one attempt to fix the "dying ReLU" problem. Instead of the function being zero when x < 0, a leaky ReLU will instead have a small negative slope (of 0.01, or so). That is, the function computes $f(x) = 1(x < 0)(\alpha x) + 1(x >= 0)(x)$ where α is a small constant. Some people report success with this form of activation function, but the results are not always consistent. The slope in the negative region can also be made into a parameter of each neuron, as seen in PReLU neurons, introduced in Delving Deep into Rectifiers, by Kaiming He et al., 2015. However, the consistency of the benefit across tasks is presently unclear.

Maxout. Other types of units have been proposed that do not have the functional form $f(w^T x + b)$ where a non-linearity is applied on the dot product between the weights and the data. One relatively popular choice is the Maxout neuron (introduced recently by Goodfellow et al.) that generalizes the ReLU and its leaky version. The Maxout neuron computes the function $\max(w_1^T x + b_1, w_2^T x + b_2)$. Notice that both ReLU and Leaky ReLU are a special case of this form (for example, for ReLU we have $w_1, b_1 = 0$). The Maxout neuron therefore enjoys all the benefits of a ReLU unit (linear regime of operation, no saturation) and does not have its drawbacks (dying

ReLU). However, unlike the ReLU neurons it doubles the number of parameters for every single neuron, leading to a high total number of parameters.

This concludes our discussion of the most common types of neurons and their activation functions. As a last comment, it is very rare to mix and match different types of neurons in the same network, even though there is no fundamental problem with doing so.

TLDR: "*What neuron type should I use?*" Use the ReLU non-linearity, be careful with your learning rates and possibly monitor the fraction of "dead" units in a network. If this concerns you, give Leaky ReLU or Maxout a try. Never use sigmoid. Try tanh, but expect it to work worse than ReLU/Maxout.

Setting up the data and the model

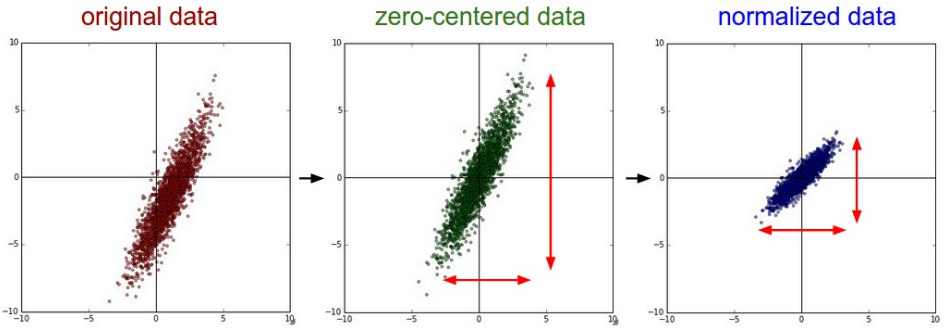
In the previous section we introduced a model of a Neuron, which computes a dot product following a non-linearity, and Neural Networks that arrange neurons into layers. Together, these choices define the new form of the **score function**, which we have extended from the simple linear mapping that we have seen in the Linear Classification section. In particular, a Neural Network performs a sequence of linear mappings with interwoven non-linearities. In this section we will discuss additional design choices regarding data preprocessing, weight initialization, and loss functions.

Data Preprocessing

There are three common forms of data preprocessing a data matrix `X`, where we will assume that `X` is of size `[N x D]` (`N` is the number of data, `D` is their dimensionality).

Mean subtraction is the most common form of preprocessing. It involves subtracting the mean across every individual *feature* in the data, and has the geometric interpretation of centering the cloud of data around the origin along every dimension. In numpy, this operation would be implemented as: `X -= np.mean(X, axis = 0)`. With images specifically, for convenience it can be common to subtract a single value from all pixels (e.g. `X -= np.mean(X)`), or to do so separately across the three color channels.

Normalization refers to normalizing the data dimensions so that they are of approximately the same scale. There are two common ways of achieving this normalization. One is to divide each dimension by its standard deviation, once it has been zero-centered: (`X /= np.std(X, axis = 0)`). Another form of this preprocessing normalizes each dimension so that the min and max along the dimension is -1 and 1 respectively. It only makes sense to apply this preprocessing if you have a reason to believe that different input features have different scales (or units), but they should be of approximately equal importance to the learning algorithm. In case of images, the relative scales of pixels are already approximately equal (and in range from 0 to 255), so it is not strictly necessary to perform this additional preprocessing step.



Common data preprocessing pipeline. **Left**: Original toy, 2-dimensional input data. **Middle**: The data is zero-centered by subtracting the mean in each dimension. The data cloud is now centered around the origin. **Right**: Each dimension is additionally scaled by its standard deviation. The red lines indicate the extent of the data - they are of unequal length in the middle, but of equal length on the right.

PCA and Whitening is another form of preprocessing. In this process, the data is first centered as described above. Then, we can compute the covariance matrix that tells us about the correlation structure in the data:

```
# Assume input data matrix X of size [N x D]
X -= np.mean(X, axis = 0) # zero-center the data (important)
cov = np.dot(X.T, X) / X.shape[0] # get the data covariance matrix
```

The (i,j) element of the data covariance matrix contains the *covariance* between i-th and j-th dimension of the data. In particular, the diagonal of this matrix contains the variances. Furthermore, the covariance matrix is symmetric and positive semi-definite. We can compute the SVD factorization of the data covariance matrix:

```
U,S,V = np.linalg.svd(cov)
```

where the columns of `U` are the eigenvectors and `S` is a 1-D array of the singular values. To decorrelate the data, we project the original (but zero-centered) data into the eigenbasis:

```
Xrot = np.dot(X, U) # decorrelate the data
```

Notice that the columns of `U` are a set of orthonormal vectors (norm of 1, and orthogonal to each other), so they can be regarded as basis vectors. The projection therefore corresponds to a rotation of the data in `X` so that the new axes are the eigenvectors. If we were to compute the covariance matrix of `Xrot`, we would see that it is now diagonal. A nice property of `np.linalg.svd` is that in its returned value `U`, the eigenvector columns are sorted by their eigenvalues. We can use this to reduce the dimensionality of the data by only using the top few eigenvectors, and discarding the dimensions along which the data has no variance. This is also sometimes refereed to as Principal Component Analysis (PCA) dimensionality reduction:

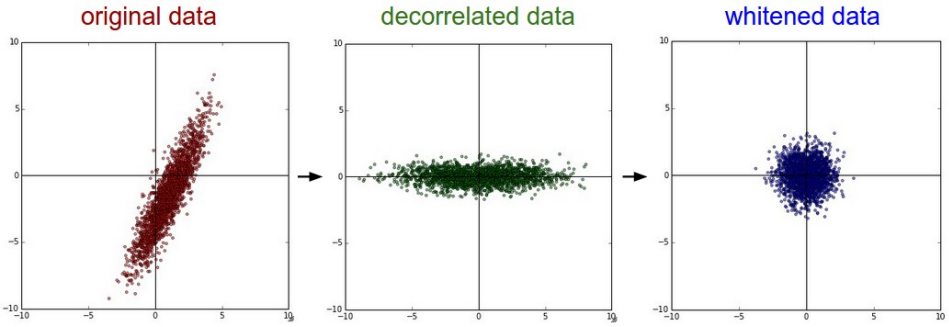
```
Xrot_reduced = np.dot(X, U[:,:100]) # Xrot_reduced becomes [N x 100]
```

After this operation, we would have reduced the original dataset of size [N x D] to one of size [N x 100], keeping the 100 dimensions of the data that contain the most variance. It is very often the case that you can get very good performance by training linear classifiers or neural networks on the PCA-reduced datasets, obtaining savings in both space and time.

The last transformation you may see in practice is **whitening**. The whitening operation takes the data in the eigenbasis and divides every dimension by the eigenvalue to normalize the scale. The geometric interpretation of this transformation is that if the input data is a multivariable Gaussian, then the whitened data will be a Gaussian with zero mean and identity covariance matrix. This step would take the form:

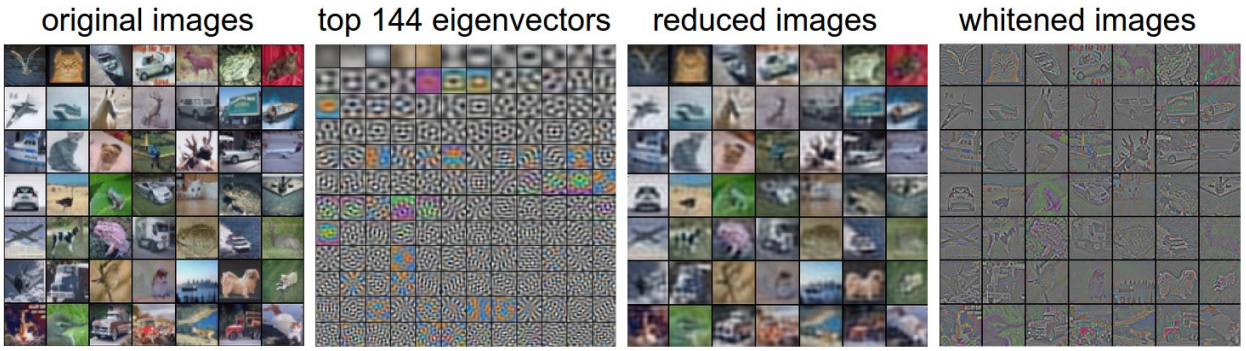
```
# whiten the data:
# divide by the eigenvalues (which are square roots of the singular values)
Xwhite = Xrot / np.sqrt(S + 1e-5)
```

Warning: Exaggerating noise. Note that we're adding 1e-5 (or a small constant) to prevent division by zero. One weakness of this transformation is that it can greatly exaggerate the noise in the data, since it stretches all dimensions (including the irrelevant dimensions of tiny variance that are mostly noise) to be of equal size in the input. This can in practice be mitigated by stronger smoothing (i.e. increasing 1e-5 to be a larger number).



PCA / Whitening. **Left**: Original toy, 2-dimensional input data. **Middle**: After performing PCA. The data is centered at zero and then rotated into the eigenbasis of the data covariance matrix. This decorrelates the data (the covariance matrix becomes diagonal). **Right**: Each dimension is additionally scaled by the eigenvalues, transforming the data covariance matrix into the identity matrix. Geometrically, this corresponds to stretching and squeezing the data into an isotropic gaussian blob.

We can also try to visualize these transformations with CIFAR-10 images. The training set of CIFAR-10 is of size 50,000 x 3072, where every image is stretched out into a 3072-dimensional row vector. We can then compute the [3072 x 3072] covariance matrix and compute its SVD decomposition (which can be relatively expensive). What do the computed eigenvectors look like visually? An image might help:



Left: An example set of 49 images. **2nd from Left:** The top 144 out of 3072 eigenvectors. The top eigenvectors account for most of the variance in the data, and we can see that they correspond to lower frequencies in the images. **2nd from Right:** The 49 images reduced with PCA, using the 144 eigenvectors shown here. That is, instead of expressing every image as a 3072-dimensional vector where each element is the brightness of a particular pixel at some location and channel, every image above is only represented with a 144-dimensional vector, where each element measures how much of each eigenvector adds up to make up the image. In order to visualize what image information has been retained in the 144 numbers, we must rotate back into the "pixel" basis of 3072 numbers. Since U is a rotation, this can be achieved by multiplying by U.transpose()[:144,:], and then visualizing the resulting 3072 numbers as the image. You can see that the images are slightly blurrier, reflecting the fact that the top eigenvectors capture lower frequencies. However, most of the information is still preserved. **Right:** Visualization of the "white" representation, where the variance along every one of the 144 dimensions is squashed to equal length. Here, the whitened 144 numbers are rotated back to image pixel basis by multiplying by U.transpose()[:144,:]. The lower frequencies (which accounted for most variance) are now negligible, while the higher frequencies (which account for relatively little variance originally) become exaggerated.

In practice. We mention PCA/Whitening in these notes for completeness, but these transformations are not used with Convolutional Networks. However, it is very important to zero-center the data, and it is common to see normalization of every pixel as well.

Common pitfall. An important point to make about the preprocessing is that any preprocessing statistics (e.g. the data mean) must only be computed on the training data, and then applied to the validation / test data. E.g. computing the mean and subtracting it from every image across the entire dataset and then splitting the data into train/val/test splits would be a mistake. Instead, the mean must be computed only over the training data and then subtracted equally from all splits (train/val/test).

Weight Initialization

We have seen how to construct a Neural Network architecture, and how to preprocess the data. Before we can begin to train the network we have to initialize its parameters.

Pitfall: all zero initialization. Let's start with what we should not do. Note that we do not know what the final value of every weight should be in the trained network, but with proper data normalization it is reasonable to assume that approximately half of the weights will be positive and half of them will be negative. A reasonable-sounding idea then might be to set all the initial weights to zero, which we expect to be the "best guess" in expectation. This turns out to be a mistake, because if every neuron in the network computes the same output, then they will also all compute the same gradients during backpropagation and undergo the exact same parameter updates. In other words, there is no source of asymmetry between neurons if their weights are initialized to be the same.

Small random numbers. Therefore, we still want the weights to be very close to zero, but as we have argued above, not identically zero. As a solution, it is common to initialize the weights of the neurons to small numbers and refer to doing so as *symmetry breaking*. The idea is that the neurons are all random and unique in the beginning, so they will compute distinct updates and integrate themselves as diverse parts of the full network. The implementation for one weight matrix might look like `W = 0.01* np.random.randn(D,H)`, where `randn` samples from a zero mean, unit standard deviation Gaussian. With this formulation, every neuron's weight vector is initialized as a random vector sampled from a multi-dimensional Gaussian, so the neurons point in random direction in the input space. It is also possible to use small numbers drawn from a uniform distribution, but this seems to have relatively little impact on the final performance in practice.

Warning: It's not necessarily the case that smaller numbers will work strictly better. For example, a Neural Network layer that has very small weights will during backpropagation compute very small gradients on its data (since this gradient is proportional to the value of the weights). This could greatly diminish the "gradient signal" flowing backward through a network, and could become a concern for deep networks.

Calibrating the variances with 1/sqrt(n). One problem with the above suggestion is that the distribution of the outputs from a randomly initialized neuron has a variance that grows with the number of inputs. It turns out that we can normalize the variance of each neuron's output to 1 by scaling its weight vector by the square root of its *fan-in* (i.e. its number of inputs). That is, the recommended heuristic is to initialize each neuron's weight vector as: `w = np.random.randn(n) / sqrt(n)`, where `n` is the number of its inputs. This ensures that all neurons in the network initially have approximately the same output distribution and empirically improves the rate of convergence.

The sketch of the derivation is as follows: Consider the inner product $s = \sum_i^n w_i x_i$ between the weights w and input x, which gives the raw activation of a neuron before the non-linearity. We can examine the variance of s:

$$\begin{aligned}
\mathrm{Var}(s) &= \mathrm{Var}(\sum_i^n w_i x_i) \\
&= \sum_i^n \mathrm{Var}(w_i x_i) \\
&= \sum_i^n [E(w_i)]^2 \mathrm{Var}(x_i) + [E(x_i)]^2 \mathrm{Var}(w_i) + \mathrm{Var}(x_i)\mathrm{Var}(w_i) \\
&= \sum_i^n \mathrm{Var}(x_i)\mathrm{Var}(w_i) \\
&= (n\mathrm{Var}(w))\,\mathrm{Var}(x)
\end{aligned}$$

where in the first 2 steps we have used properties of variance. In third step we assumed zero mean inputs and weights, so $E[x_i] = E[w_i] = 0$. Note that this is not generally the case: For example ReLU units will have a positive mean. In the last step we assumed that all w_i, x_i are identically distributed. From this derivation we can see that if we want s to have the same variance as all of its inputs x, then during initialization we should make sure that the variance of every weight w is $1/n$. And since $\text{Var}(aX) = a^2\text{Var}(X)$ for a random variable X and a scalar a, this implies that we should draw from unit gaussian and then scale it by $a = \sqrt{1/n}$, to make its variance $1/n$. This gives the initialization `w = np.random.randn(n) / sqrt(n)`.

A similar analysis is carried out in Understanding the difficulty of training deep feedforward neural networks by Glorot et al. In this paper, the authors end up recommending an initialization of the form $\text{Var}(w) = 2/(n_{in} + n_{out})$ where n_{in}, n_{out} are the number of units in the previous layer and the next layer. This is based on a compromise and an equivalent analysis of the backpropagated gradients. A more recent paper on this topic, Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification by He et al., derives an initialization specifically for ReLU neurons, reaching the conclusion that the variance of neurons in the network should be $2.0/n$. This gives the initialization `w = np.random.randn(n) * sqrt(2.0/n)`, and is the current recommendation for use in practice in the specific case of neural networks with ReLU neurons.

Sparse initialization. Another way to address the uncalibrated variances problem is to set all weight matrices to zero, but to break symmetry every neuron is randomly connected (with weights sampled from a small gaussian as above) to a fixed number of neurons below it. A typical number of neurons to connect to may be as small as 10.

Initializing the biases. It is possible and common to initialize the biases to be zero, since the asymmetry breaking is provided by the small random numbers in the weights. For ReLU non-linearities, some people like to use small constant value such as 0.01 for all biases because this ensures that all ReLU units fire in the beginning and therefore obtain and propagate some gradient. However, it is not clear if this provides a consistent improvement (in fact some results seem to indicate that this performs worse) and it is more common to simply use 0 bias initialization.

In practice, the current recommendation is to use ReLU units and use the `w = np.random.randn(n) * sqrt(2.0/n)`, as discussed in He et al..

Batch Normalization. A recently developed technique by Ioffe and Szegedy called Batch Normalization alleviates a lot of headaches with properly initializing neural networks by explicitly forcing the activations throughout a network to take on a unit gaussian distribution at the beginning of the training. The core observation is that this is possible because normalization is a simple differentiable operation. In the implementation, applying this technique usually amounts to insert the BatchNorm layer immediately after fully connected layers (or convolutional layers, as we'll soon see), and before non-linearities. We do not expand on this technique here because it is well described in the linked paper, but note that it has become a very common practice to use Batch Normalization in neural networks. In practice networks that use Batch Normalization are significantly more robust to bad initialization. Additionally, batch normalization can be interpreted as doing preprocessing at every layer of the network, but integrated into the network itself in a differentiable manner. Neat!