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Advanced methods in Machine Learning
Assignment 2

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Contents

1 Recurrent Models for MNIST

1.1 Understanding LSTM vs GRU

We specify the LSTM and GRU cells and recurrence equations.

LSTM

$$f_t = \sigma_g(W_f x_t + U_f h_{t-1} + b_f) \tag{1}$$
$$i_t = \sigma_g(W_i x_t + U_i h_{t-1} + b_i) \tag{2}$$
$$o_t = \sigma_g(W_o x_t + U_o h_{t-1} + b_o) \tag{3}$$
$$c_t = f_t \odot c_{t-1} + i_t \odot \sigma_g(W_c x_t + U_c h_{t-1} + b_c) \tag{4}$$
$$h_t = o_t \odot \tanh(c_t) \tag{5}$$

where σ_g is the sigmoid activation function.

GRU

$$z_t = \sigma_g(W_z x_t + U_z h_{t-1} + b_z) \tag{6}$$
$$r_t = \sigma_g(W_r x_t + U_r h_{t-1} + b_r) \tag{7}$$
$$h = \tanh(W_h x_t + U_f(h_{t-1} \odot r_t) + b_h) \tag{8}$$
$$h_t = (1 - z_t) \odot h + z_t \odot h_{t-1} \tag{9}$$

We also note that any composition of affine transformations and the sigmoid functions in these cases never lead to inverses of the sigmoid functions, and only the case of $\sigma(constant)$ leads to linearity.

(a) Reframing the question: define the LSTM cell to be a function $h_t = g_\Theta(x_t)$, where Θ are all of the parameters of the LSTM cell, $\{W, U, b\}_{f,i,o,c}$. Similarly for the GRU cell. We are trying to find parameters that in general make the equivalence

$$h_t = x_t = g_\Theta(x_t) \tag{10}$$

true. Since this implies that $g_\Theta = Id$ which is linear, linearity is a necessary condition for this to be true. Hence if we can show that linearity doesn't hold in general, or that the only linear case is independent of x_t (i.e. constant with regards to x_t) then this also implies that $h_t \neq x_t$ in general.

LSTM We consider $g_\Theta =: g$ and try to find Θ that makes g linear. Since

$$h_t = o_t \odot \sigma_h(c_t)$$

We need both o_t and $\sigma_h(c_t)$ to be linear in x_t. This in turn implies that c_t is constant with respect to x_t since else the whole thing is non-linear. Similarly as

$$o_t = \sigma_g(W_o x_t + U_o h_{t-1} + b_o)$$

we need this to be constant in x_t as else it is non-linear. But this means that both o_t, c_t are constant with respect to x_t which implies that h_t doesn't depend on x_t, which means that g_Θ can't be the identity function of x_t. So we have shown that this is not possible for LSTM.

However, if we take the limit case where the sigmoid function can take on the values 0 and 1, and tanh the values -1 and 1 (done by letting the bias term b go to $\pm\infty$ elementwise to the same limit), we can 'store' the input value x_t but only through the non-linear layer. This can be done by setting $W_o = I, U_o = 0, b_o = 0$, and $f_t, i_t = 0$ by letting $b_i, b_f \to -\infty$, then $h_t = \sigma(x_t)$. In general we have a map from two spaces which are of different dimensions, so an identity in this case is not possible.

GRU Similarly as to the LSTM we have the relation

$$h_t = g_\Theta(x_t) = (1 - z_t) \odot h + z_t \odot h_{t-1}$$

reasoning as in the case with LSTM, we need both terms of the addition to be linear, the necessary condition. We have the two terms $(1 - z_t) \odot h$ and $z_t \odot h_{t-1}$. Since z_t is a non-linear function in x_t or constant in x_t and h_{t-1} is independent of x_t we must be able to kill off the terms that lead to a non-linear function in x_t. We see that since h_{t_1} is given and assumed equal to x_{t-1} that $z_t = 0$ which implies that we must have

$$h_t = h = \tanh(W_h x_t + U_f(h_{t-1} \odot r_t) + b_h)$$

But this is either constant or non-linear in x_t hence it can't the be identity function. So we have shown that this is not possible for GRU.

Interpreting storing as in h_t only depending on x_t, we can do that by letting $z_t = 0$ by letting $b_z \to -\infty$ setting $W_z, U_z = 0$ and setting $U_h, b_h = 0, W_h = I$, meaning that $h_t = \tanh(x_t)$.

(b) **LSTM** We want to show that there is a configuration such that $c_t = c_{t-1}$. This is simply done by setting $i_t = 0, f_t = 1$ by letting $W_i, U_i = 0, b_i \to -\infty$ and $W_f, U_f = 0, b_f \to \infty$.

GRU For the GRU we can make $h_t = h_{t-1}$ by setting the $z_t = 1$ by letting $W_z, U_z = 0, b_z \to \infty$. Then $h_t = 0 \odot h + h_{t-1} = h_{t-1}$.

(c) We define a shorthand for the notation of an affine transformation as

$$A_l(x_t, h_{t-1}) = W_l x_t + U_l h_{t-1} + b_l$$

With this we note that we can decompose the output and state for the LSTM and GRU as

LSTM

$$\begin{aligned} h_t &= \sigma(A_o(x_t, h_{t-1})) \odot \\ &\quad (\sigma(\sigma(A_f(x_t, h_{t-1})) \odot c_{t-1} + \sigma(A_i(x_t, h_{t-1})) \odot \tanh(A_c(x_t, h_{t-1})))) \\ &\quad = \sigma(A_o(x_t, h_{t-1})) \odot \sigma(\sigma(A_f(x_t, h_{t-1})) \odot c_{t-1} + \sigma(A_i(x_t, h_{t-1})) \odot \tanh(A_c(x_t, h_{t-1})))) \end{aligned}$$

GRU

$$\begin{aligned} h_t &= \tanh(A_h(x_t, h_{t-1} \odot \sigma(A_r(x_t, h_{t-1})))) \\ &\quad - \tanh(A_h(x_t, h_{t-1} \odot \sigma(A_r(x_t, h_{t-1})))) \odot \sigma(A_z(x_t, h_{t-1})) \\ &\quad + \sigma(A_z(x_t, h_{t-1})) \odot h_{t-1} \end{aligned}$$

We now construct a counter-example showing that the GRU is not a special case of the LSTM. Consider the scalar case. Let A_z be zero, A_h be such that $W_h = 1, U_h = 1, b_h = 1$, equally for A_r. This gives us that

$$h_t = 0.5 \tanh(x_t + h_{t-1}\sigma(x_t + h_{t-1} + 1) + 1) + 0.5h_{t-1}$$

We see that the LSTM can never have this form since we have a sigmoid function inside of the tanh function which doesn't exist for the LSTM. Thus the GRU is not in general a special case of the LSTM.

2 Task 1: Classification

For task 1 I implemented a python file called `task1.py`. By design you pass to this function several command line arguments which lets you pick the architectures that we are interested in. The differences in all of the models have to do with either the cell type used in the RNN part of the network (LSTM or GRU) or the innards of the cell (32, 64, 128 or 3 stacks of 32 for the hidden unit). Finally we also have to fix the first part of the output network (the feed forward part of the whole architectures) since it has to map the output to the assumed 100 dimensions after the first layer. Since my design takes all models into consideration, what I will describe below applies to all models of task 1. All of this was done using the functions in tensorflow, and this was done for all architectures and models in this assignment.

The models mainly differ in their expressive power, since a higher number of hidden units in the RNN gives a bigger space of functions that the whole network can represent it should be able to learn more aspects of the data set. However this also means that it should be easier to overfit. The stacked layer network is somewhere in between, but should possibly be the most expressive of them all since the parameters of each layer are independent in a way that the 128 hidden units model is not.

2.1 Architecture

My architecture is straightforward, the only difference between the vanilla implementation in the notes is that for the feed forward layers, I use batch normalisation.

I used batch normalisation since this reduces the internal covariate shift at each layer. Essentially, models are able to learn patterns much better if the input distribution of each layer is the same during training. For deep models it is common that as we use backpropagation and change the parameters of the shallow layers, the distribution of the input of the deeper layers change. Batch normalisation mitigates this by normalising the input. In our case, I used batch normalisation before the input to the affine layers in the final part of the network, the feed-forward network following the recurrent neural network part. Thus my architecture includes two instances of batch normalisation, once directly after the output from the RNN and once after the first non-linearity in the feed-forward network.

Batch normalisation is different during training and testing as during training the normalisation is done with respect to batch mean and variance of the layer input which is dependent on how you batch your data set during training, while for testing these parameters are fixed. To get estimates of the population mean and variance of each layer input to be used during testing I kept an exponential running average of the mean and variance.

Define the index i to show belonging to layer i and letting t denote the time step of training, B_t the batch at time t. The input to layer i will have some distribution. This distribution will when we are finished with training have some population mean and variance μ^i, σ^{2i}. We then estimate these parameters to be used during test time by keeping an exponential running average. That is, if at time t we have the batch estimates of the parameters $\mu^i_{t,B}, \sigma^{2i}_{B,t}$ then we update the estimates of the population parameters, $\hat{\mu}^i_t, \hat{\sigma}^{2i}_t$ with a chosen decay rate d as

$$\hat{\mu}_t^i = d * \hat{\mu}_{t-1}^i + (1-d) * \mu_{t,B}^i$$
$$\hat{\sigma}_t^{2i} = d * \hat{\sigma}_{t-1}^{2i} + (1-d) * \sigma_{t,B}^{2i}$$

where we initialise the running averages to be

$$\hat{\mu}_0^i = 0$$
$$\hat{\sigma}_0^{2i} = 1$$

The decay rate specifies how much we take previous data into consideration and gives us a more accurate estimate given that we train long enough so that we forget the initialisations.

Running the training for a long enough time enables us to get accurate estimates of the population mean and variance. Note that in general these parameters are vectors.

During train time the batch normalisation then applies the operation to each input of batch B of layer i as

$$BN_{\gamma,\beta}(x^i) = \gamma * \frac{x^i - \mu_B^i}{\sigma_B^i} + \beta \tag{11}$$

where γ and β are vectors to be learned. This also has a regularising effect meaning that we don't have to rely on dropout to reduce overfit.[1]

Similarly is done during test, except that we know use the estimated mean and variance instead of the batch mean and variance.

The batch normalisation helps a lot, without the training is highly erratic and often resets to random prediction in terms of loss and accuracy. With batch normalisation I am able to reach much better results, in a shorter number of training steps, which reinforces the results of the paper.[2]

2.2 Hyperparameters and optmization

Before I used batch normalisation I had a hard time getting the models to train properly. After experimenting I found that ADAM seemed to yield the best training performance, both with and without batch normalisation. As ADAM is a pretty advanced optimisation algorithm which has been shown to work well on training neural networks this is no surprise as it takes into account more of the aspects of the trajectory than just SGD which just looks at the current position to calculate the next one given the learning rate and batch through the derivatives gotten from the backpropagation.

Since batch normalisation yields models which train in a much more stable manner than without it as it reduces internal covariate shift I was able to consistently get great results by using the hyperparameters of

learning rate 0.001

decay rate 0.99

[1] https://arxiv.org/abs/1502.03167
[2] https://arxiv.org/abs/1502.03167

batch size 256

This was the same for all models except for GRU with 32 hidden units of 3 layers as my computer died that I had running at home, and rerun it with 60 epochs instead.

The learning rate enables training the models until saturation and they achieved consistently increasing accuracy except for possibly 3 stacked hidden layers of 32 units each, but I am not sure if this should be the case or not since it doesn't seem clear to me if this yields a more or less flexible model compared to one hidden layer of size 128. Also, since using batch normalisation means that good results can be achieved for a bigger set of hyperparameters, I did not need to search as many alternative triplets of hyperparameters as if I had trained without batch normalisation. There is also some indication that even 100 epochs was not enough for this model to fully converge.

The decay rate doesn't really impact accuracy except for that we need the final estimates of the mean and variance of the batch normalisation operators in the neural networks to be accurate estimates of the population parameters for these layers. This is independent of the back propagation and just means that we need the number of training steps to be large enough so that the resulting estimated means and variances are able to 'forget' the starting values of these parameters. Since I trained for 100 epochs which means I did approximately 21500 training steps, 0.99 should be small enough to get away from the initialisations, but high enough to yield correct estimates.

The batch size was chosen to be reasonably big to exploit both the fact that tensorflow uses highly optimized linear algebra packages which means that we get significant speedups by processing in big batches rather than increasing the number of iterations in the train loops, but small enough such that it still is stochastic and can climb out of local minima. Since I trained my models using GPU instances on AWS, The batch size was deliberately chosen to be a multiple of 32 since this meant I could optimize the use of the GPU cache and avoid cache misses speeding up training.

I trained for each model for 100 epochs. At the end of each epoch I recorded the test and train accuracy and loss, using random batches of the train and test set of size 800. Using the test accuracy I saved the model every time the test accuracy increased compared to all the previous test accuracies during that run. This amounts to a kind of early stopping. Since I used the test set to set hyperparameters I might overfit, however, since the accuracies were stochastic this mitigates this somehow. Nevertheless I believe that the result should generalise well.

2.2.1 Graphs

We have the following graphs from training the models in task 1.[3] Note that the filled trajectories are smoothed with a smoothing value of 0.5 in tensorboard, while the shadow trajectories are the original trajectories without smoothing.

LSTM

[3]These images are sufficient to get a good overview of the training. However, they are easier to interpret interactively by running `tensorboard --logdir=./models` from the parent directory and then going to the link using Chrome.

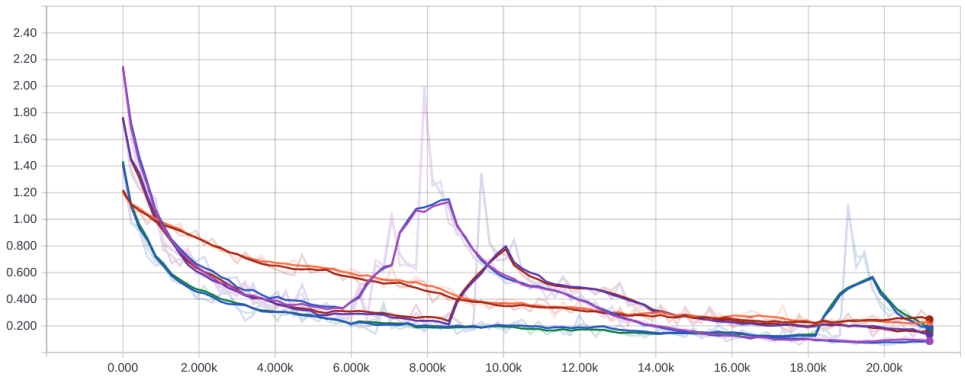


Figure 1: Cross entropy vs training steps

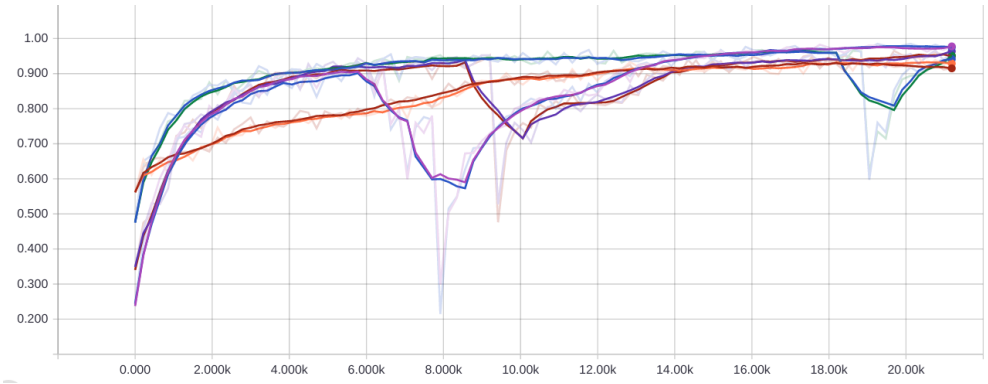


Figure 2: Accuracy vs training steps

Legend. I will list them pairwise from the lowest starting point in the accuracy graph to the highest (opposite for the graph of the loss). The first colour is the train set, second colour the test set:

Blue/Purple 128 hidden units

Red/Dark Purple 64 hidden units

Green/Blue 3 stacked layers of 32 hidden units

Orange/Red 32 hidden units

GRU

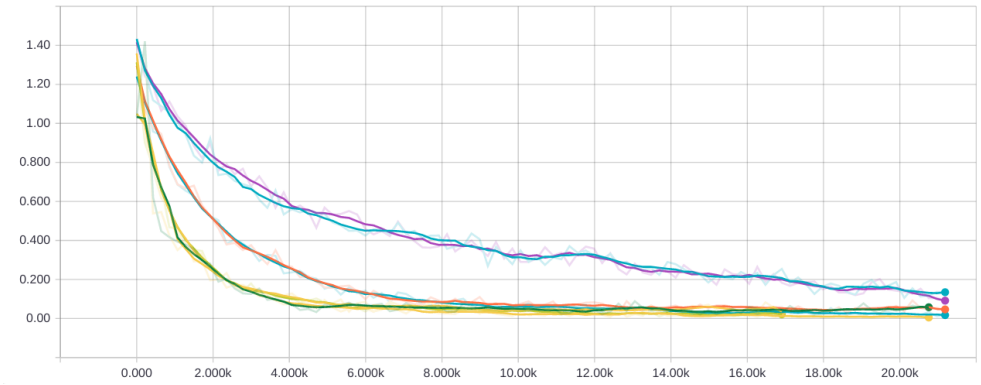


Figure 3: Cross entropy vs training steps

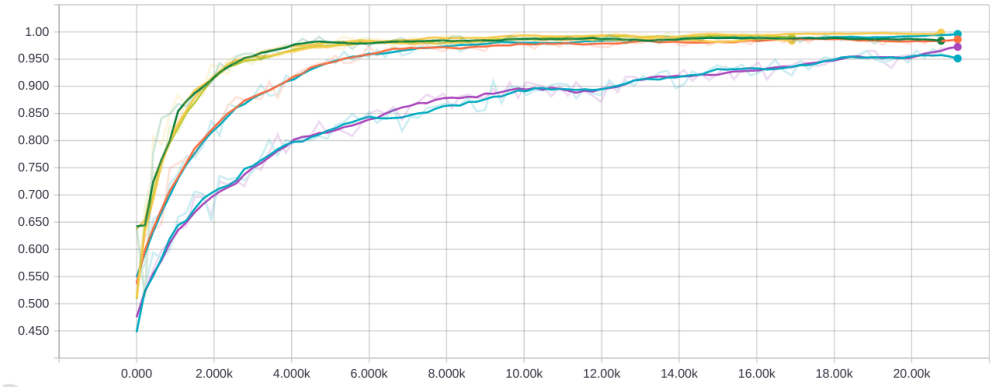


Figure 4: Accuracy vs training steps

Legend. I will list them pairwise from the lowest starting point in the accuracy graph to the highest (opposite for the graph of the loss). The first colour is the train set, second colour the test set:

Dark Purple/Cyan 32 hidden units

Gold/Yellow 64 hidden units

Purple/Cyan 3 stacked layers of 32 hidden units

Green/Yellow 128 hidden units

Comparing these graphs for LSTM and GRU, we see that while both seem to converge over enough epochs, the GRU's have a much more stable training than the LSTM's, and much better end results as can bee seen in the results section.. Naturally the results will fluctuate somehow, and since I take stochastic estimations of accuracy and loss at the end of each epoch, this is not surprising. However, I did not think that there would be such a massive difference as we can see from the graphs. If we look at the shadow trajectories of the LSTM's we note that several of the trajectories drop from a good result down to almost baseline accuracy/loss. This influenced my decision to use GRU's in task 2 since they seem better fit to the task. I don't know if this can be generalised beyond these architectures/data set.

From the graph we can see that there is an improvement in the accuracy/loss as the number of hidden units increases, but the 3 stacked layers of 32 hidden unit cells falls in between, possibly as it converges much more slowly than the rest. However, in order to conclude this we should collect data over several runs to make sure that this i not a statistical fluke.

2.3 Results

Model: LSTM	(1 layer, 32 units)	(1 layer, 64 units)	(1 layer, 128 units)	(3 layers, 32 units)
Testing Loss	0.25888	0.20495	0.23591	0.46100
Training Loss	0.26707	0.19597	0.24081	0.45192
Testing Accuracy	0.92130	0.94180	0.93150	0.85900
Training Accuracy	0.91827	0.94342	0.93053	0.86185

Model: GRU	(1 layer, 32 units)	(1 layer, 64 units)	(1 layer, 128 units)	(3 layers, 32 units)
Testing Loss	0.15829	0.05887	0.05793	0.08601
Training Loss	0.16102	0.03587	0.03767	0.06462
Testing Accuracy	0.95240	0.98310	0.98180	0.97550
Training Accuracy	0.95136	0.98796	0.98709	0.97975

Comparing this to the result in assignment one we get that these are slightly worse in general than the network which saw the whole image at once. This is to be expected since even though RNN's have a way to store previous information in the input sequence, it still can't see the whole image at once and get a holistic overview like in assignment 1. However, I think if I used batch normalisation in assignment 1 and 2 compared to just in assignment 2 here, the differences would be more pronounced.

3 Task 2: Pixel prediction

Similarly to task 1 I made the python file `task2a.py` able to train all the different models (32, 64, 128, 3 stacks of 32) by choosing arguments from the command line. I chose the GRU's since my experiments and plots from task 1 showed me that GRU's gave a higher accuracy for both training and test set and a much more consistent training trace than LSTM's which was more choppy and occasionally well into training dropped back to a performance equivalent to random initialization. Additionally, this suggests that LSTM's are much more prone to destroying the learned patterns when ADAM updates the parameters than the GRU cell.

The same analysis as in task 1 applies here:

The models mainly differ in their expressive power, since a higher number of hidden units in the RNN gives a bigger space of functions that the whole network can represent it should be able to learn more aspects of the data set. However this also means that it should be easier to overfit. The stacked layer network is somewhere in between, but should possibly be the most expressive of them all since the parameters of each layer are independent in a way that the 128 hidden units model is not.

3.1 Architecture

The architecture is very similar to that of Task 1. The difference is that instead of using the many-to-one RNN as in task 1 we are using a many-to-many architecture. This is done by getting the output at each point and running it through an affine layer which maps it down from the number of hidden units to a scalar which is then squashed, equivalent to logistic regression. This number is then interpreted as the probability of the next pixel being filled in. Using this probability vector where the i'th entry corresponds to the probability over the $i+1$'th pixel, we can use the original input vector as our output vector by slicing it from the second to the last element. This lets us calculate the average cross entropy per pixel which we can use backpropagation on to learn the optimal parameters of the model.

I didn't use any batch normalisation in task 2 since it worked fine without it.

3.2 Hyperparameters

The hyperparameters chosen mimics that of task 1. I ran the models for 50 epochs since they converged much faster than in task 1.

We have the following hyperparameters for all of the models

learning rate 0.001

batch size 256

The hyperparameters were chosen for the same reason as in task 1. A 0.001 learning rate worked perfect for all models and gave a smooth trajectory and good final performance. I saved the models every time the test accuracy went below the best accuracy so far for each epoch. This possibly meant I overfit, but it looks like it will give good generalisation performance.

The batch size was chosen to be big enough to take advantage of the vectorisation and GPU's on AWS but small enough to be a source of stochasticity meaning that we don't get stuck in local minima as easily.

3.2.1 Graphs

We have the following graphs from training the models in task 2.[4] Note that the filled trajectories are smoothed with a smoothing value of 0.5 in tensorboard, while the shadow trajectories are the original trajectories without smoothing.

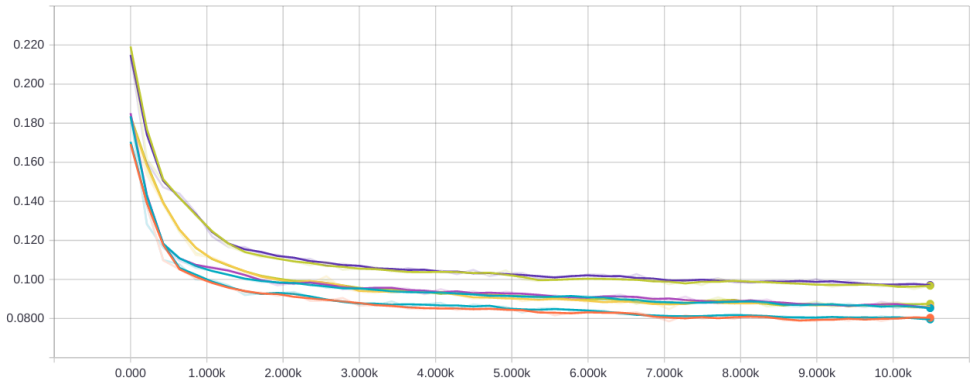


Figure 5: Cross entropy vs training steps (GRU)

[4]These images are sufficient to get a good overview of the training. However, they are easier to interpret interactively by running `tensorboard --logdir=./models` from the parent directory and then going to the link using Chrome.

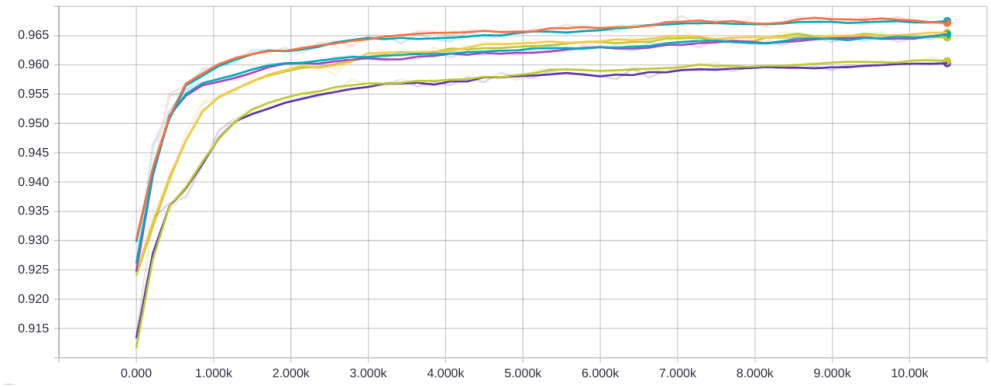


Figure 6: Accuracy vs training steps (GRU)

Legend. I will list them pairwise from the lowest starting point in the accuracy graph to the highest (opposite for the graph of the loss). The first colour is the train set, second colour the test set:

Dark Purple/Gold 32 hidden units

Gold/Yellow 64 hidden units

Purple/Cyan 3 stacked layers of 32 hidden units

Cyan/Orange 128 hidden units

Conclusion about the performance of the different models mirror the conclusions of task 1.

3.3 Results

Model: GRU	(1 layer, 32 units)	(1 layer, 64 units)	(1 layer, 128 units)	(3 layers, 32 units)
Testing Loss	0.09659	0.08784	0.08092	0.08532
Training Loss	0.09744	0.08867	0.08154	0.08610

3.4 Cross-entropies

Using the code as specified in `task2b.py` we calculate the average per-pixel cross-entropy averaged over the 10 generated inpaintings of the set of 100 masked images from the test set (The normal cross entropy, ground truth or inpaintings, for one image is reported as an average over the inpainted masked pixels, we then produce 1000 images, 10 generated samples per image sampled from the test set. Finally we average the pixel cross-entropy over all of the 100*10=1000 images).

3.4.1 Tables

GRU 32	Ground Truth	Inpaintings
1 pixel	0.17033	0.14874
10 pixels	0.38597	0.20815
28 pixels	0.21755	0.12829
300 pixels	0.79950	0.09417

GRU 64	Ground Truth	Inpaintings
1 pixel	0.16718	0.17623
10 pixels	0.35977	0.19590
28 pixels	0.20932	0.12678
300 pixels	0.60323	0.07297

GRU 128	Ground Truth	Inpaintings
1 pixel	0.16667	0.13610
10 pixels	0.29943	0.18597
28 pixels	0.18047	0.12209
300 pixels	0.53247	0.06623

GRU 3 stacked 32	Ground Truth	Inpaintings
1 pixel	0.15753	0.17612
10 pixels	0.36390	0.18387
28 pixels	0.20713	0.11607
300 pixels	0.69276	0.07297

3.4.2 Comparison of the models

We have the same kind of comparison as in task 1. Due to the increased expressive power, as we trained the

3.5 Interesting inpaintings

For the inpaintings I observed that numbers which are distinct (1, 4, 0) were more often filled in correctly than numbers which are ambiguous (2, 3, 5, 6, 8, 9). However, we have an additional source of noise since the binarization sometimes leave us with ambiguous representations of the original image due to how it thresholds.

All the images are arranged such that from left to right we have

1. Original image
2. Masked image
3. Sample 1
4. Sample 2
5. Sample 3
6. Sample 4
7. Sample 5

3.5.1 10 pixels inpaintings

(a) 32 GRU

(b) 64 GRU

(c) 128 GRU

(d) 3 stack 32 GRU

Figure 7: Digit A

(a) 32 GRU

(b) 64 GRU

(c) 128 GRU

(d) 3 stack 32 GRU

Figure 8: Digit B

(a) 32 GRU

(b) 64 GRU

(c) 128 GRU

(d) 3 stack 32 GRU

Figure 9: Digit C

3.5.2 28 pixels inpaintings

(a) 32 GRU

(b) 64 GRU

(c) 128 GRU

(d) 3 stack 32 GRU

Figure 10: Digit A

(a) 32 GRU

(b) 64 GRU

(c) 128 GRU

(d) 3 stack 32 GRU

Figure 11: Digit B

(a) 32 GRU

(b) 64 GRU

(c) 128 GRU

(d) 3 stack 32 GRU

Figure 12: Digit C

3.5.3 300 pixels inpaintings

(a) 32 GRU

(b) 64 GRU

(c) 128 GRU

(d) 3 stack 32 GRU

Figure 13: Digit A

(a) 32 GRU

(b) 64 GRU

(c) 128 GRU

(d) 3 stack 32 GRU

Figure 14: Digit B

(a) 32 GRU

(b) 64 GRU

(c) 128 GRU

(d) 3 stack 32 GRU

Figure 15: Digit C

4 Task 3: In-painting

4.1 Results

(a) We have a probability distribution over the pixels in an image given by the model, where the value of the i'th pixel is denoted by $x_t \in \{0, 1\}$. We denote the quantity $P(x_t = 1|x_{1:t-1}) = p_t$, i.e. the probability of a pixel being filled in (equal to 1, black). This also means that we can write $P(x_t = 0|x_{1:t-1}) = 1-p_t$ and thus that

$$P(x_t|x_{1:t-1}) = p_t^{y_t}(1 - p_t)^{1-y_t}$$

where $y_t = I(x_t = 1)$. Equally this means that

$$\log(P(x_t|x_{1:t-1})) = y_t \log(p_t) + (1 - y_t) \log(1 - p_t)$$

We are looking to find the probability given by our model over the missing pixels (1 or a patch of 4), i.e

$$P(X|I \setminus X)$$

where X is the set of missing pixels and I is all of the pixels in the image. We let the number of pixels in an image be denoted T and note that the probability of a pixel can only start from $t = 2$ since our model only predict pixels given at least one starting input.

1 Pixel Let the missing pixel be τ then the value of this pixel is x_τ. We have the following given the values of the other pixels in the image

$$\begin{aligned}
P(x_\tau|x_{1:\tau-1}, x_{\tau+1:T}) &= \frac{P(x_\tau, x_{1:\tau-1}, x_{\tau+1:T})}{P(x_{1:\tau-1}, x_{\tau+1:T})} \\
&= K'P(x_\tau, x_{1:\tau-1}, x_{\tau+1:T}) \\
&= K\prod_{t=2}^{T} P(x_t|x_{1:t-1}) \\
&= K(\prod_{t=2}^{\tau-1} P(x_t|x_{1:t-1}))P(x_\tau|x_{1:\tau-1})(\prod_{\tau+1}^{T} P(x_T|x_{1:T-1}))
\end{aligned}$$

where $K = \frac{P(x_1)}{P(x_{1:\tau-1}, x_{\tau+1:T})} > 0$.

Hence we have found the probability of x_τ given the rest of the pixels as a function of the value of x_τ. We note that maximizing this is equivalent to minimizing the cross entropy as

$$\begin{aligned}
\arg\max_{x_\tau} P(x_\tau|x_{1:\tau-1}, x_{\tau+1:T}) &= \arg\max_{x_\tau} \log\left(\prod_{t=2}^{T} P(x_\tau|x_{1:\tau-1}, x_{\tau+1:T})\right) \\
&= \arg\max_{x_\tau} \sum_{t=2}^{T} (y_t \log(p_t) + (1 - y_t)\log(1 - p_t)) \\
&= \arg\min_{x_\tau} \sum_{t=2}^{T} -(y_t \log(p_t) + (1 - y_t)\log(1 - p_t)) \\
&= \arg\min_{x_\tau} \textit{Cross-Entropy}(y, p)
\end{aligned}$$

where y and p are the vectors filled with y_t respectively p_t.

2x2 patch of pixels Let the missing pixels be indexed by $\tau_1, \tau_2, \tau_3, \tau_4$, we want to find

$$\begin{aligned}
P(x_{\tau_1}, x_{\tau_2}, x_{\tau_3}, x_{\tau_4}|x_t \in I \setminus \{x_{\tau_1}, x_{\tau_2}, x_{\tau_3}, x_{\tau_4}\}) &= \frac{P(x_t \in I)}{P(x_t \in I \setminus \{x_{\tau_1}, x_{\tau_2}, x_{\tau_3}, x_{\tau_4}\})} \\
&= K\prod_{t=2}^{T} P(x_t|x_{1:t-1})
\end{aligned}$$

From here we see that this is equivalent to the one-pixel case except for that the K is different and that the function depends on 4 rather than one variable. This means that to find the maximizer of this probability we have to find the quadruplet that minimize the cross entropy

$$\underset{x_{\tau_1}, x_{\tau_2}, x_{\tau_3}, x_{\tau_4}}{\arg\min} \quad \textit{Cross-entropy}(y, p)$$

(b) Using the fact from above I could easily get the optimal inpaintings. Using this I calculated data and statistics. I used the GRU 128 hidden units model from task 2 since this gave the best result when predicting the pixels in task 2.

4.1.1 1 pixel inpainting

We have the following histograms and statistics of the cross-entropies over the 1000 images

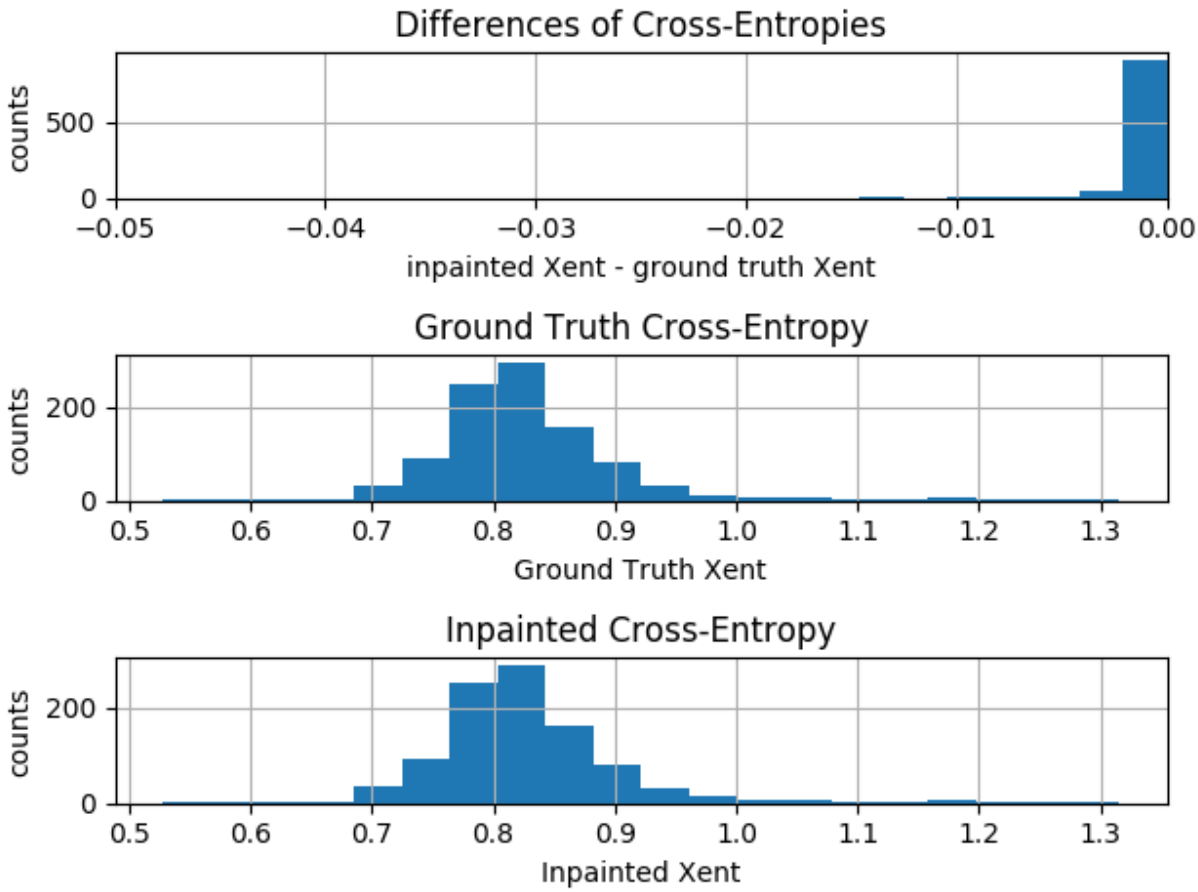


Figure 16: Cross entropy histograms, 1 pixel patch

Cross entropy	Ground Truth	Inpaintings	Difference
Mean	0.83094	0.82982	-0.00112
Standard deviation	0.08606	0.08436	0.00909

4.1.2 2x2 pixels inpainting

We have to following histograms of the cross-entropies over the 1000 images

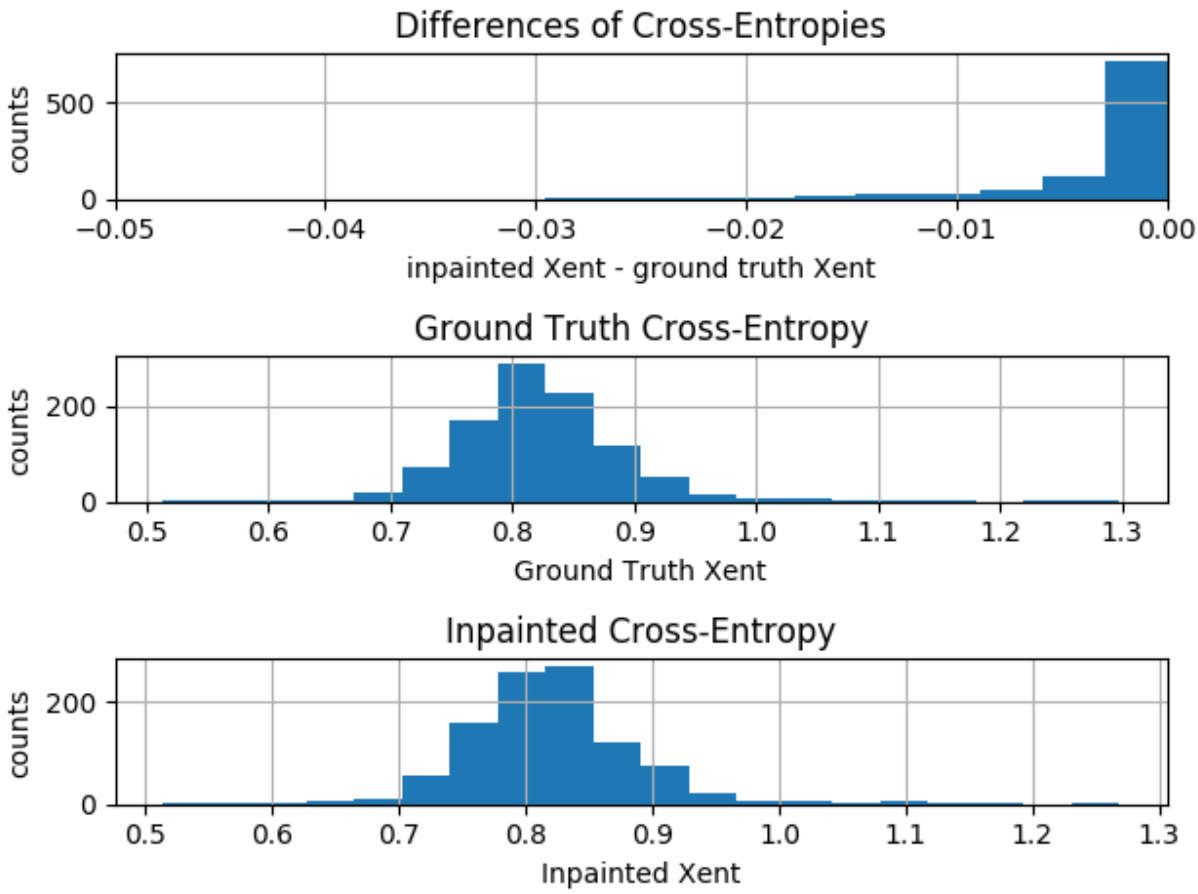


Figure 17: Cross entropy histograms, 2 by 2 pixel patch

Cross entropy	Ground Truth	Inpaintings	Difference
Mean	0.82615	0.82206	-0.00409
Standard deviation	0.07245	0.06932	0.01523

4.1.3 Analysis

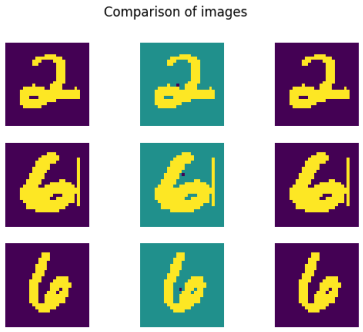
Comparing the histograms and cross entropy means and standard deviations we see that the difference in the cross entropy of the ground truth image and the optimal inpainted images are very low, majority of them between 0.001 and 0 distance from each other. However, there are certain outliers (which still aren't very big, but further away than the bulk). I set the x-limit of the x-axis to be smaller so that the peak around 0 became more prominent, but meaning that a few outliers are outside the diagram for both 1 and 2 by 2 pixel patches.

The reason for why inpaintings always have a lower cross entropy than the ground truth is simple. As we test all of the different possible binary patches and taking the minimum as the inpainting, we will have that since the ground truth is equal to one of these patches that the cross entropy of the inpainting will be less or equal to the cross entropy of the ground truth. In reality, the in painting cross entropies that are far from the ground truth cross entropies reflect the shortcomings of the model.

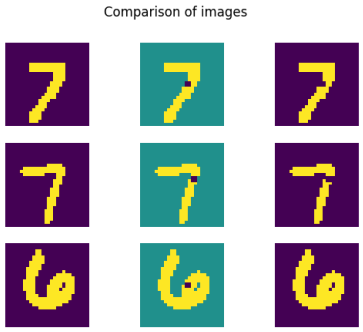
If we compare between the 1 pixel and 2 by 2 pixel patches we see that the 1 pixel patch we see that the

only real difference is that for just one pixel to inpaint, we get a zero difference much more often. This simply means that for fewer pixels, the model guess right more often as there are fewer combinations to actually guess (2 vs 16). This is reflected in the mean and standard deviation of the differences between the ground truth and inpainted cross entropy, where the mean is closer to 0 and standard deviation is smaller for the 1 pixel inpainting.

4.1.4 Example inpaintings



(a) 1 Pixel patch inpainting



(b) 16 Pixel patch inpainting

Figure 18: In order: Ground Truth, Masked, Inpainting. Rows specify index of image set.

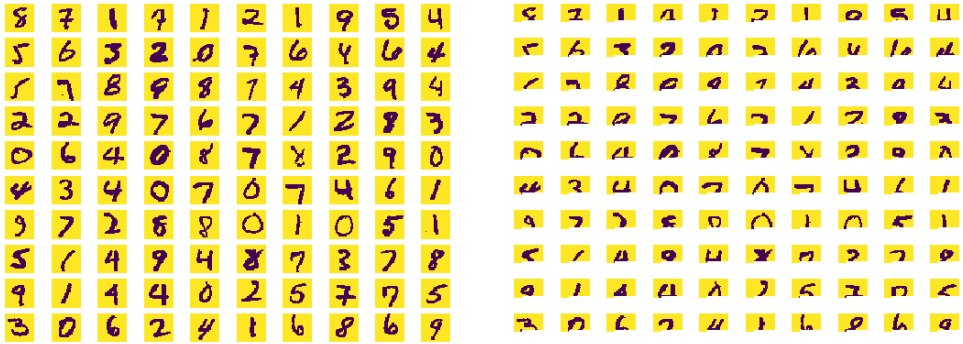
4.1.5 Saved .npy arrays

The saved inpaintings can be located in the directory relative to the parent directory, `./code/data/inpainting_data/`, and are called `optimal_inpaintings_1pixel_patch.npy` and `optimal_inpaintings_2x2pixel_patch.npy`.

A task 2 images

A.1 generated images

A.1.1 ground truth and masked images

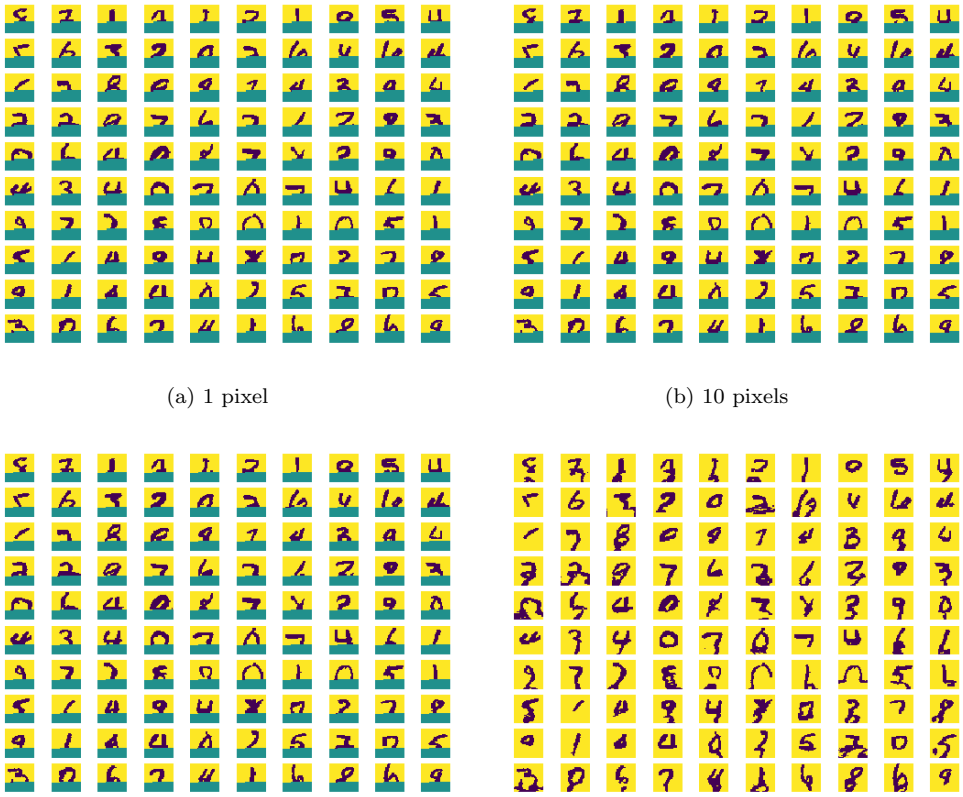


(a) Ground truth

(b) Masked

Figure 19: Ground truth and masked images sampled from the test set

A.1.2 32 hidden units



(a) 1 pixel

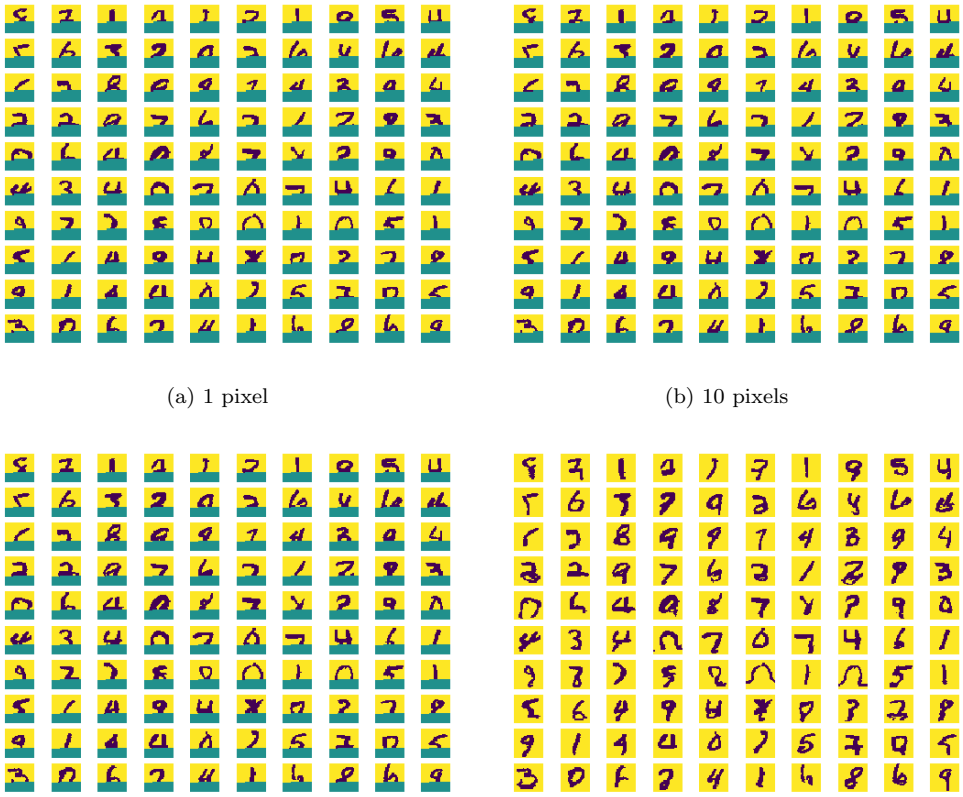
(b) 10 pixels

(c) 28 pixels

(d) 300 pixels

Figure 20: first generated sample of each of the hundred test set images

A.1.3 64 hidden units



(a) 1 pixel

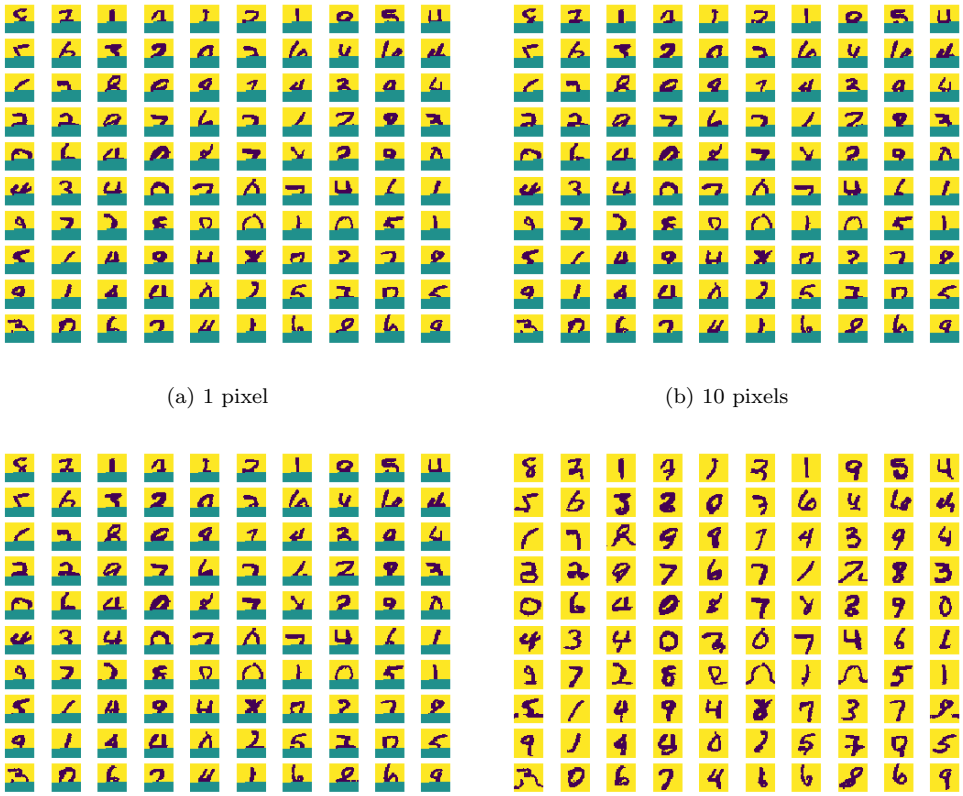
(b) 10 pixels

(c) 28 pixels

(d) 300 pixels

Figure 21: first generated sample of each of the hundred test set images

A.1.4 128 hidden units



(a) 1 pixel

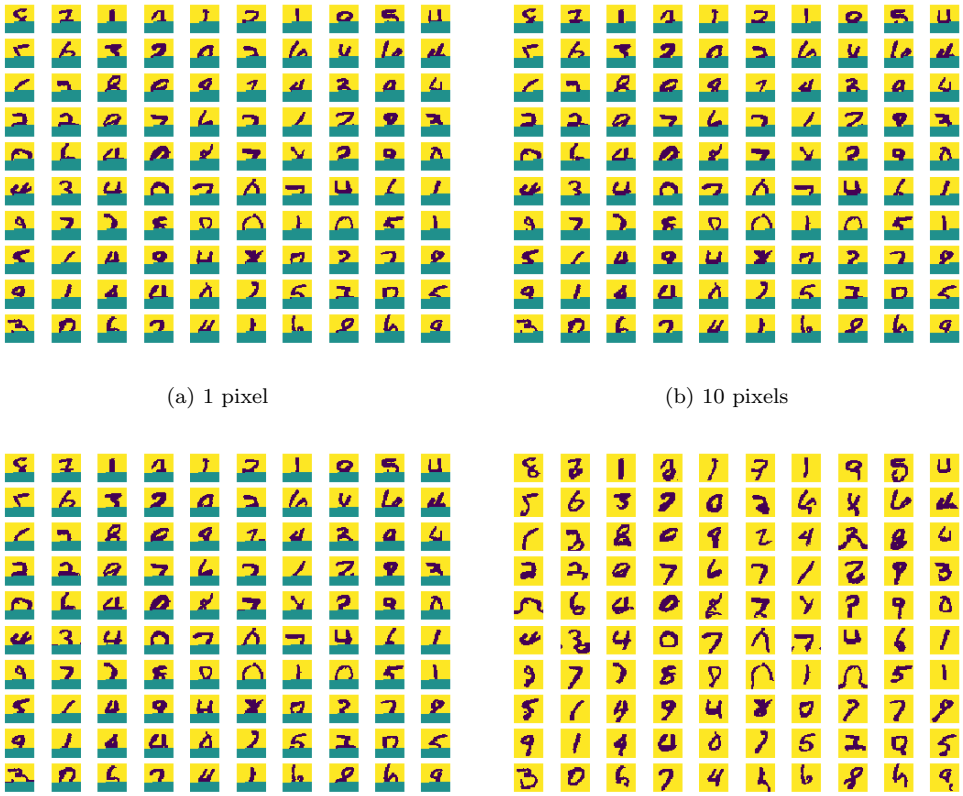
(b) 10 pixels

(c) 28 pixels

(d) 300 pixels

Figure 22: first generated sample of each of the hundred test set images

A.1.5 3 stacked layers of 32 hidden units



(a) 1 pixel

(b) 10 pixels

(c) 28 pixels

(d) 300 pixels

Figure 23: first generated sample of each of the hundred test set images