AM160 Final Project

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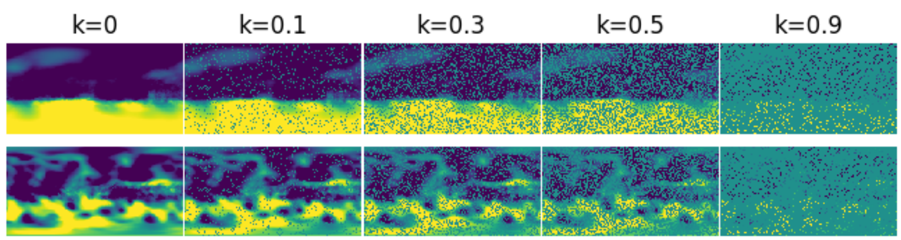
The code for this project can be found on colab. I included some fun interactive graphs there too!

1 Denoising VAE

The purpose of this part was to implement a VAE that takes sparse weather data and produces an estimate of the actual weather data. Here is an example of the sparsification function I used:



I tried to implement this two ways, first with a model that just tries to fill in points where the data is sparse (like a derivative model for a differential equation), and also a model that simply outputs the unsparsified data. The second model turned out to be much better, however I included both in this report :)

1.1 Model hyperparameters

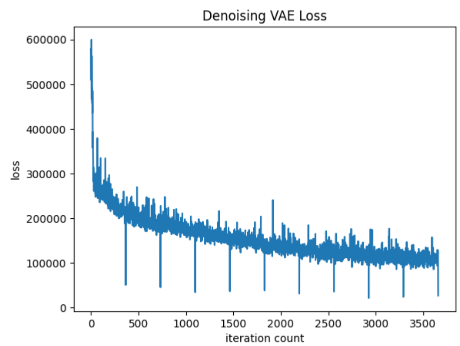
The VAE I used for all problems in this final was the same: 2 2-d convolutional layers to two linear layers to get the latent space mean and variance for the encoder, and a linear layer to get from latent space into 2 2-d convolutional layers to get the output! I programmed the latent space to be variable in length. For the denoising VAE, I included a conditioning in the decoder on the sparsity level for my final product, however I learned this didn't matter too much. For both models here, the latent dimension was 200.

1.2 Derivative model

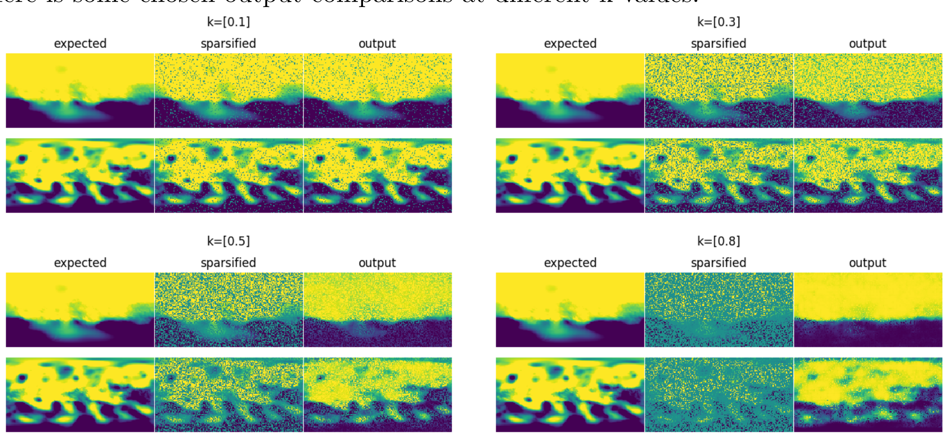
To train the model, I used 10 epochs with batch sizes of 16. For each batch, I chose a random k to sparsify the data. The loss function was MSE loss + KL divergence. The expected output of the model was filled-in values at the sparse points, so in order to get a desparsified output

$$x_{\text{desparsified}} = M(x_{\text{sparsified}}) + x_{\text{sparsified}}$$

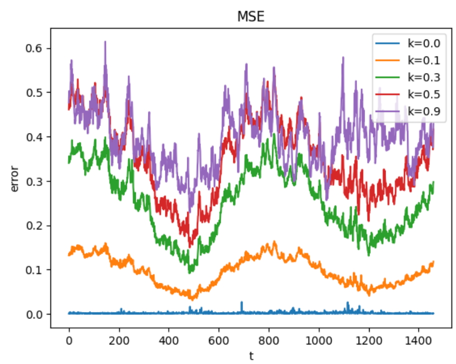
Here is a loss graph:



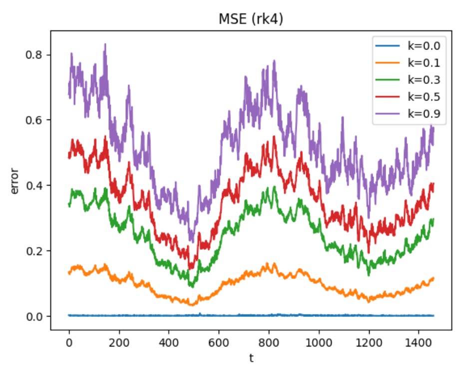
Here is some chosen output comparisons at different k values:



And an error graph over t for different k-values.



just for fun, I wanted to see if I could use an rk4 step to get better results instead of just adding the model's output (which would be an euler step). It was not better :(

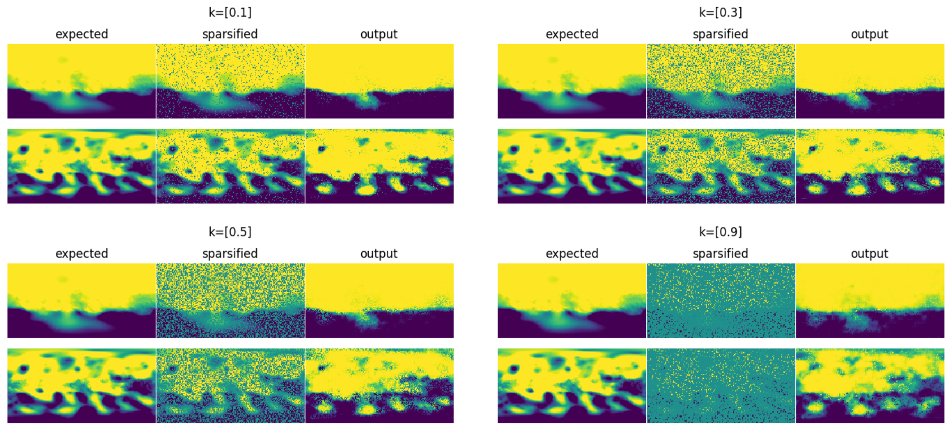


1.3 Direct model

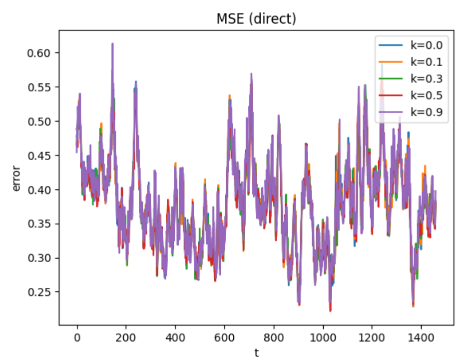
Instead of doing the derivative model, the simpler direct model is better for this case! Here, we cirectly calculate the desparsified data. Additionally, we conditioned the model on the k-value.

$$x_{\text{desparsified}} = M(x_{\text{sparsified}}, k)$$

The output is much better:



Interestingly, the error doesn't change much with differing k values any more! This means the conditioning really works!



2 Autoregressive Generative VAE

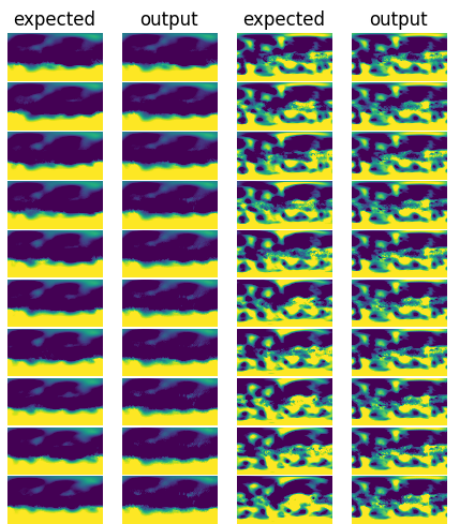
For this problem, I accidentally implemented it incorrectly! I was not concatenating x_{t-1} to the latent space of the decoder, instead I was inputting it into the VAE overall! I fixed this, but I included that incorrect implementation in this writeup because I put some work into it...

2.1 Incorrect implementation

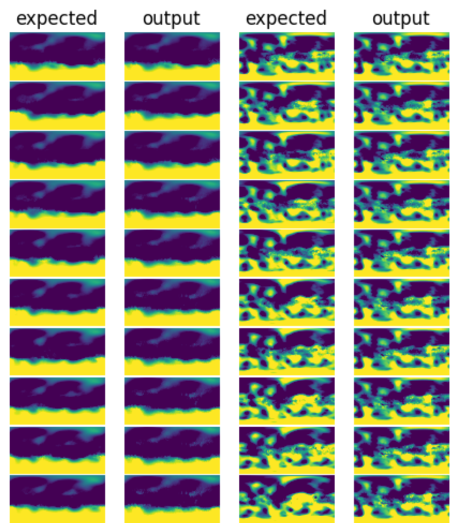
I tried to make a diffusion model for this problem but I got kind of confused. It turns out my generative VAE model workes pretty well, despite fast (¡2min) training times! Additionally, prediction times are pretty fast too. To create the generative model, I used the same VAE as in the previous section. The decoder was conditioned on x_{t-1} AND a random variable r which was only 1-dimensional. I used a derivative model, where the model predicts the change in state between timesteps, as trying to just output the next step wasn't working very well at all. The latent dimension for this part was much larger than above, around 1000 long.

$$\frac{dx}{dt}|_{x_{t+1}} = M(x_t)$$

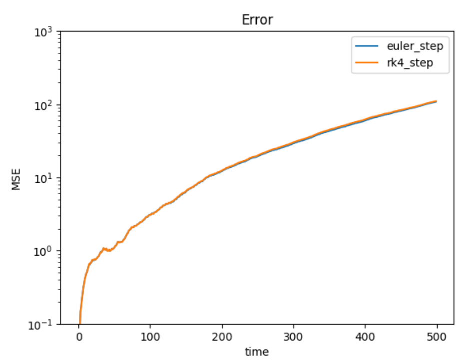
Also, because the decoder is conditioned on a random r, we can take an ensemble of samples at every timestep and find the mean of that ensemble to get the mean output! This made the iteration much more stable. For the step function, I implemented both rk4 and euler steps, however both were just about equivalent so if I were to actually use this model I'd use the euler step (much less overhead). Iterating for 500 steps was still super fast! Only taking $\tilde{3}0$s despite 10 samples per rk4 step and 4 rk4 steps per full step! Here is the euler-step output plotted for the first 10 timesteps:



And here's the RK4 output:

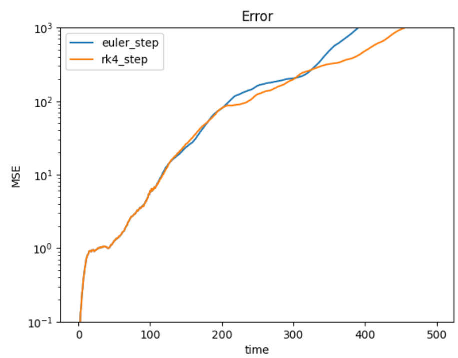


The MSE graph was pretty nice too! <1 MSE up to 50 iterations. That's almost 2 weeks of output! Pretty sweet....

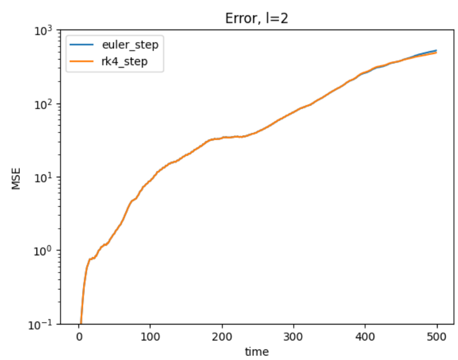


2.2 Correct implementation

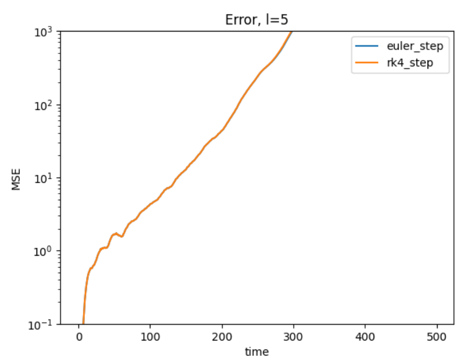
The correct implementation was to train just the decoder, given noise concatenated with the previous timestep for the input to the decoder. Like above, I chose to use a derivative model, predicting the change in the next timestep. When only training the model using the last timestep, we get slightly dissappointing results:



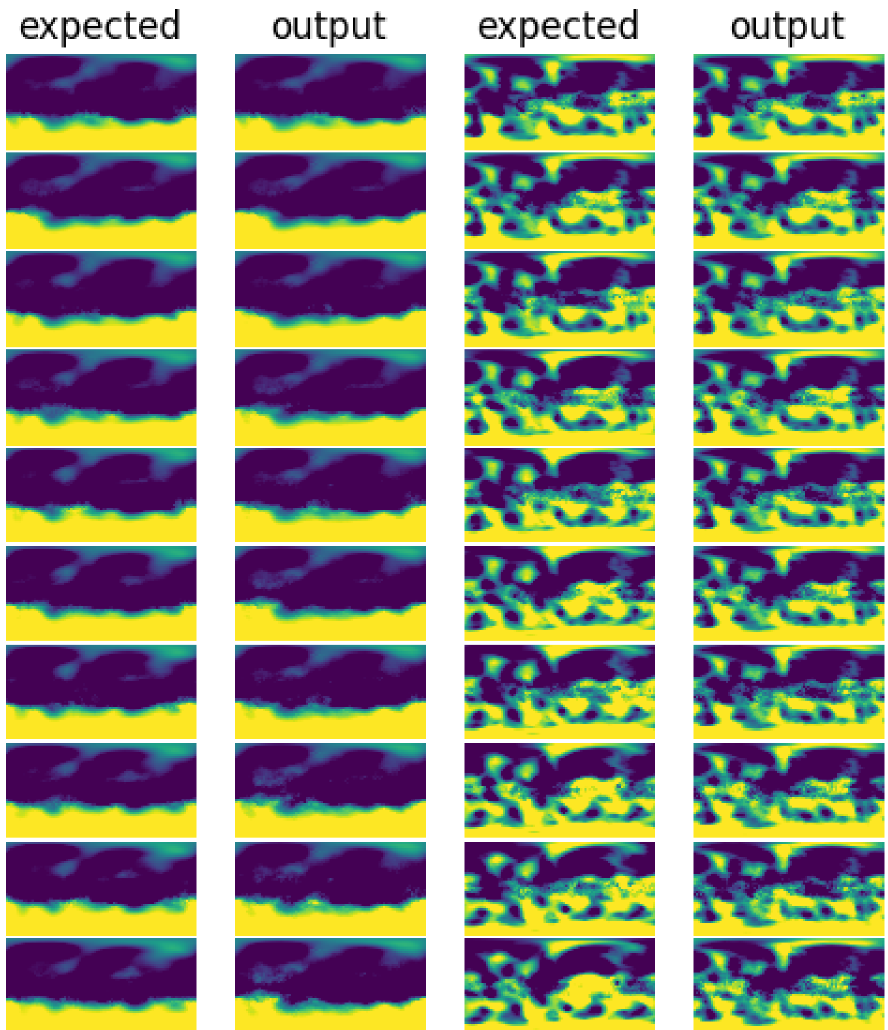
however, the beauty of this model is you can add more previous timesteps easily! Here's the error plot with the previous 2 timesteps as input:



And here's for 5:



As you can see, none of these error plots show better performance than the incorrect implementation above... I bet I could get the performance of the $l = 5$ case to be better if I had more resources to train it, however it was already taking around 5 minutes to train the model so I skipped that. Because for $l = 2$ the euler step is just about equivalent to the rk4 step, here's a comparison of the output with euler step:



2.3 Comparison

As you can see from the graphs, the "incorrect" implementation where you input x_{t-1} into a full VAE and concatenate noise to the latent dimension to create an ensemble was actually better than concatenating x_{t-1} to random noise in the latent space and decoding that! Not only does it have better error rates, it is easier to train and faster! If I were to guess why, I don't have enough parameters in my correct implementation model to train it well. Unfortunately, when I tried to increase the number of parameters I was running out of memory... Additionally, looking at both implementations it is clear that overall rk4 and euler step is nearly identical, with rk4 being slightly better usually. I'd say, for these models it doesn't make sense to use an rk4 step because it's 4x the work for really negligible impacts.

3 Forward Diffusion Process

$$
\begin{aligned}
x(t) &= \sqrt{1-\beta_t}x(t-1) + \sqrt{\beta_t}N(0,I) \\
&= \sqrt{1-\beta_t}(\sqrt{1-\beta_{t-1}}x(t-2) + \sqrt{\beta_{t-1}}N(0,I)) + \sqrt{\beta_t}N(0,I) \\
&= \sqrt{1-\beta_t}\sqrt{1-\beta_{t-1}}x(t-2) + (\sqrt{1-\beta_t}\sqrt{\beta_{t-1}} + \sqrt{\beta_t})N(0,I) \\
&\dots \\
&= x(0)\prod_{k=1}^{t}\sqrt{1-\beta_k} + N(0,I)\sum_{k=1}^{t}\sqrt{\beta_k}\prod_{j=k+1}^{t}\sqrt{1-\beta_j}
\end{aligned}
$$

We know that

$$\lim_{t\to\infty}\prod_{k=1}^{t}\sqrt{1-\beta_k} = 0$$

Additionally, we can see that

$$\sum_{k=1}^{t}\sqrt{\beta_k}\prod_{j=k+1}^{t}\sqrt{1-\beta_j}$$

always exists even as $t \to \infty$, so $x(t)$ is the sum of gaussians when t is very large. The sum of gaussians is also gaussian, so $x(t)$ approaches a gaussian.