ECE695 – ILGM

1. Kalman Filter with Neural Networks
2. Variational Autoencoders with Normalizing Flows

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Kalman Filter with Nueral Network

Motivation

- Current research in studying the optimization subspace in gradient descent.
- Came across this paper [1], One line summary:

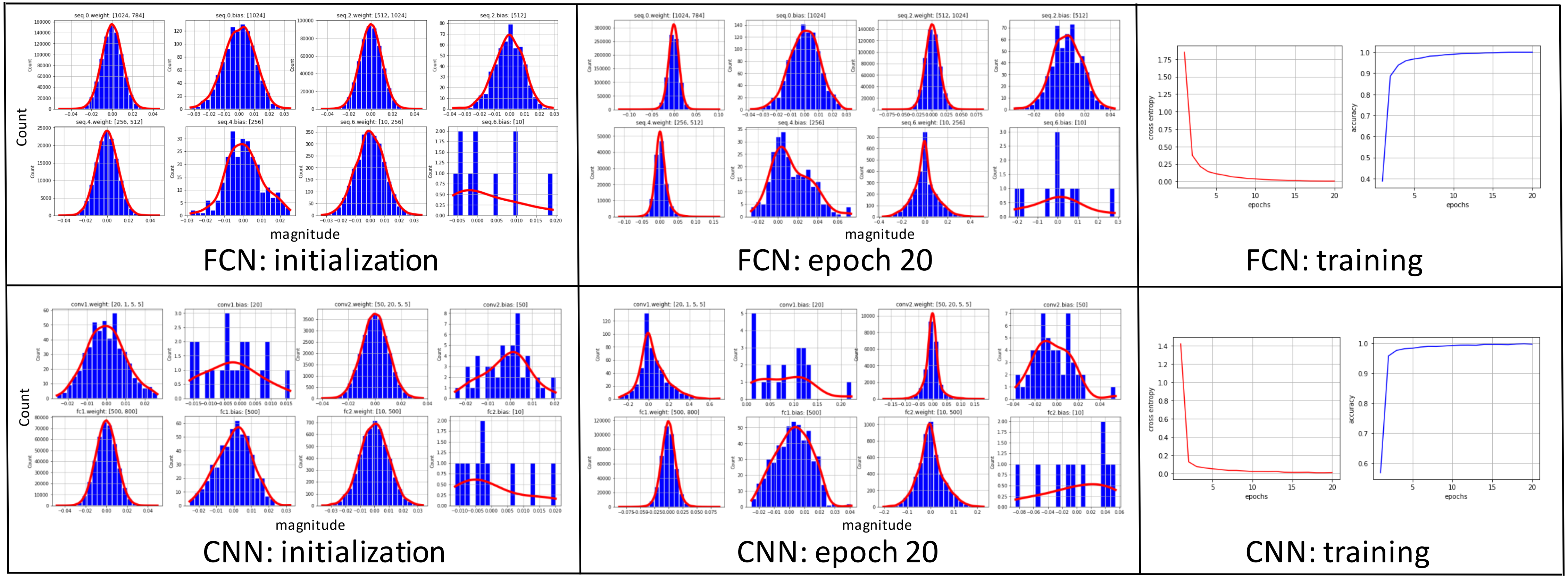
  "gradient descent tell us more than what we care about".
- Idea:
  - Neural Networks (NN) fail with confidence, i.e., false predictions with high confidence.
  - Solutions to this generally involves ensembling of multiple models trained independently.
  - In the optimization process of NNs, we discard the steps taken and only store the end weights.
  - Proposal: The path taken by the optimization can help us learn distribution of weights.
  - The parameter distribution can help us draw several models.
  - So basically, we can try to do a Bayesian prediction using NNs.

$$\underbrace{q(X_{n+1}|\theta^*)}_{\text{Frequentist}} \quad \textbf{vs} \quad \underbrace{\int_\theta q(X_{n+1}|\theta)q(\theta|x)d\theta}_{\text{Bayesian}}$$

Reference: Franchi, Gianni, et al. "TRADI: Tracking deep neural network weight distributions." *ECCV 2020*.

Neural Network Training

- Often NNs initialized using standard Gaussian distributions, $\theta_0 \sim \mathcal{N}(\mu_{\theta_0}, \sigma^2_{\theta_0})$.
- Training NN with gradient descent is a linear update: $\theta_{k+1} = \theta_k - \eta \cdot \nabla f_{\theta_k}(X, Y)$.
- A Gaussian distributed RV undergoing a linear (affine) transformation gives another Gaussian.



HMM of Weights: Kalman Filter

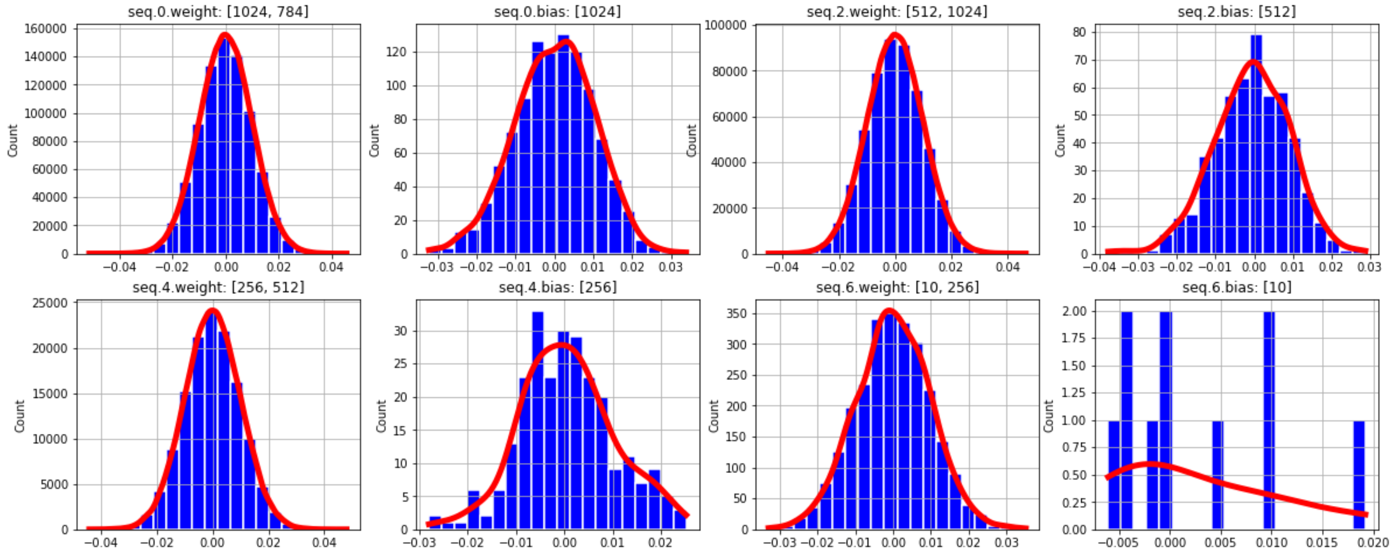
- Means of the weights follow a Markov process:

$$\mu_{k+1} = \mu_k - \mathbb{E}[\eta \cdot \nabla f_{\theta_k}(X, Y)]$$

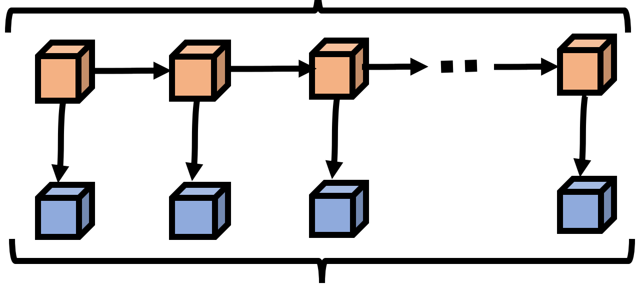
- Similarly, variance of weights can be modelled:

$$\sigma_{k+1}^2 = \sigma_k^2 + \eta^2 \mathbb{E}[(\nabla f_{\theta_k})^2] - \eta^2 \mathbb{E}^2[\nabla f_{\theta_k}]$$

- Tracking the means becomes a direct application of Kalman filtering in this case.
- Since the emissions are Gaussian distributed we get a recursive solution for tracking the means and variance.
- Simplifying assumptions:
  - Weights in different layers are independent of each other
  - Weights within the same layer can be considered pairwise related in which case it is possible to track the covariance matrix.



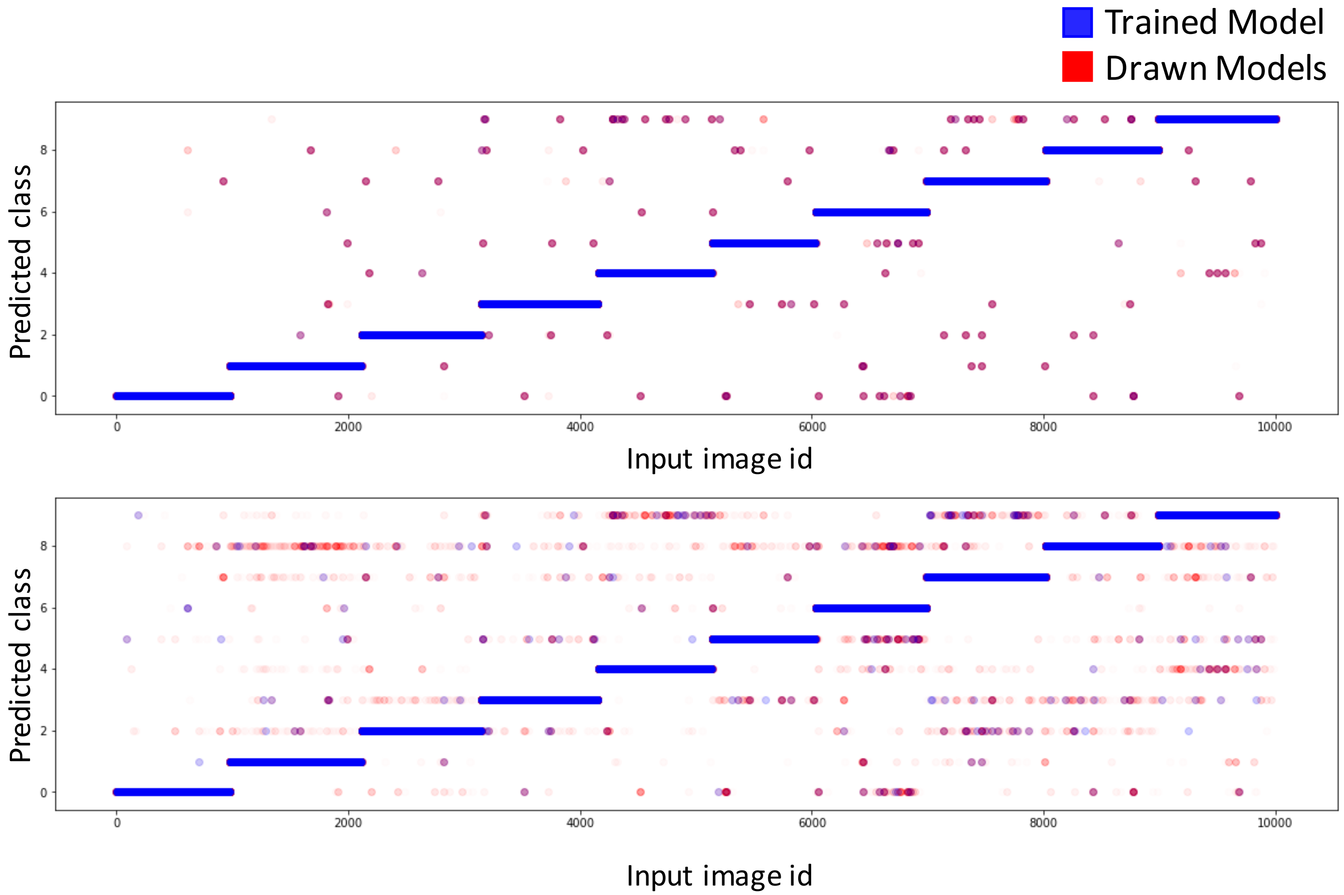
$$\mathcal{N}(\mu_{\theta_k}, \sigma_{\theta_k}^2)$$



$$\theta_k; k = 0, 1, 2, \cdots K$$

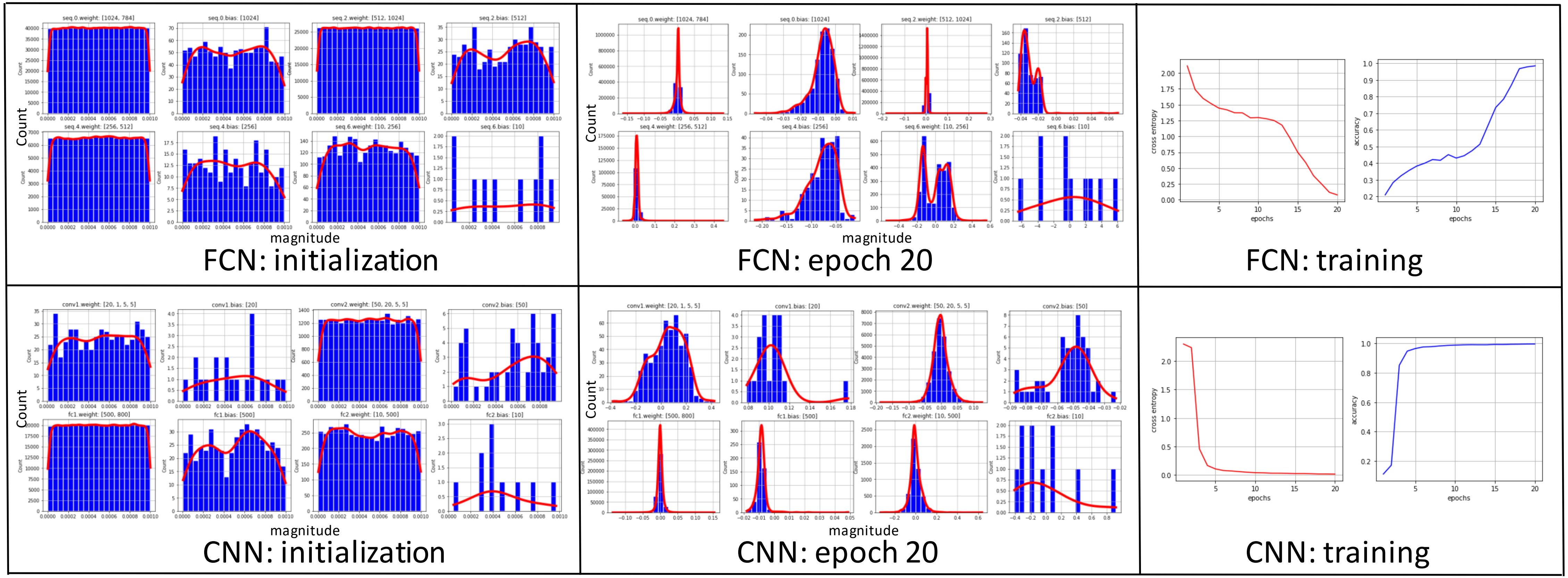
Some Results: Kalman Filter

- Trained model gives the frequentist prediction
- Models drawn from the probabililty distribution give better picture about the uncertainty in prediction.
- Classification on noisy data (bottom graph) gives a good picture of uncertainty in prediction.
- Can be used to detect out of distribution samples by checking the variance in prediction.
- There are other methods like deep-ensemble, MC Dropout methods in the same domain.
- Memory requirement of saving ensembles is higher than weight distribution tracking.



Non-Gaussian Weight Initialization

- NNs can also be initialized using non-Gaussian distributions.
- Simple case of uniform distribution. Final distributions are non-Gaussian like.
- Kalman-Filter could be replaced with Particle filter instead but computation overhead will add.

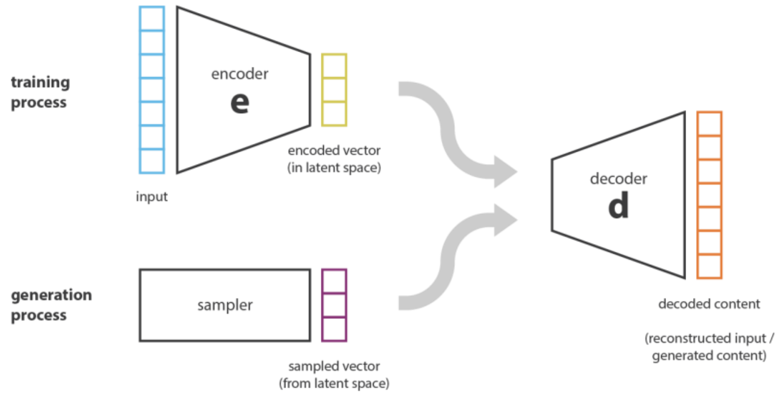


Summary

- It is possible to extract more information from gradient descent than just final weights.
- Kalman filtering gives an effective way for tracking the distribution since weight updates follow a Markov process.
- This is an alternative to ensembling as it helps us draw multiple models from the weight distribution and tends to perform better than deep ensemble and MC dropout methods.
- Compared to deep ensembles the memory footprint of this method is much less and hence practical.
- It can also be used to detect the confidence in prediction by checking the variance of prediction from different drawn models.
- This can further be extended to detection of out of sample data.

Variational Autoencoder with Normalizing Flow

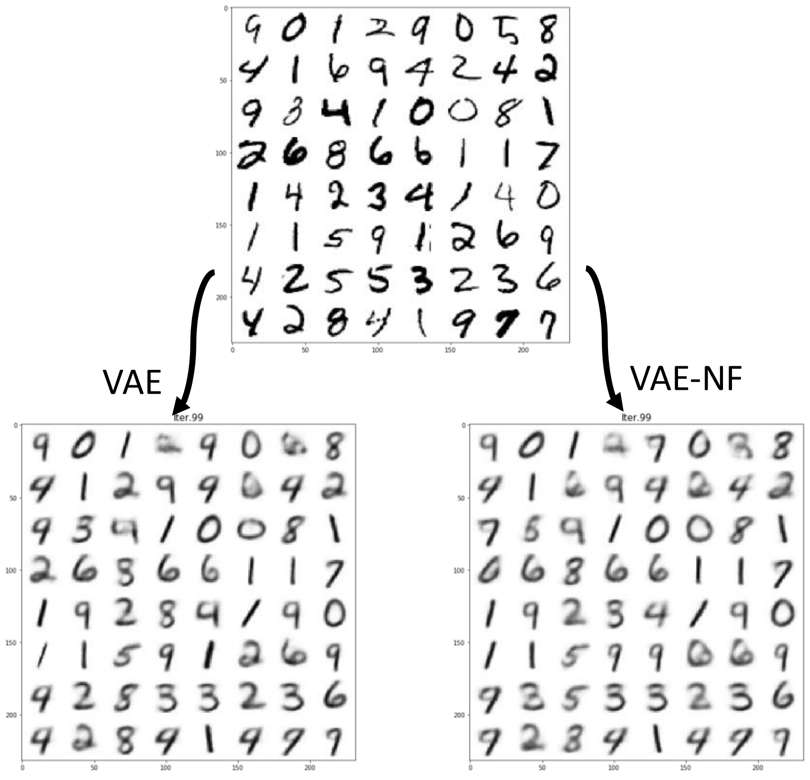
Normalizing Flows with VAE



$$\underbrace{\mathbb{E}_{r(X|Y)}[-log\, q(X|Y)]}_{\text{Reconstruction loss}} - D_{KL}[r(X|Y;\phi)||q(X;\theta)]$$

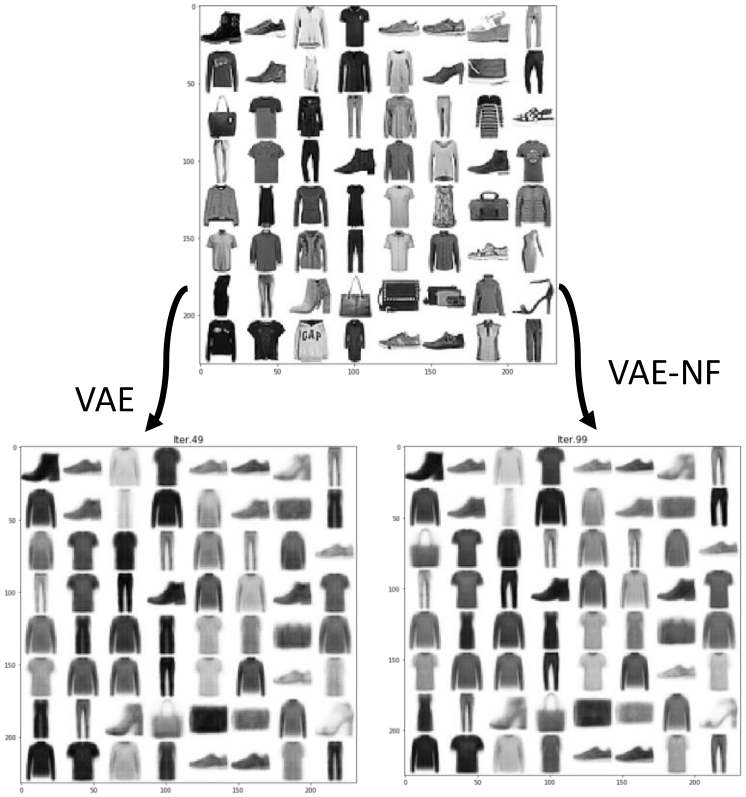
VAE: The posterior is approximated with a shifted and scaled Gaussian (decouples sampling and X).
Normalizing flows can relax this simplification!!!

$$\mathbb{E}_r[log\, r(X|Y) - log\, q(X,Y)] = \mathbb{E}_r[\underbrace{log\, q_K(X_K)}_{\text{Flow Output}} - log\, q(X,Y)]$$

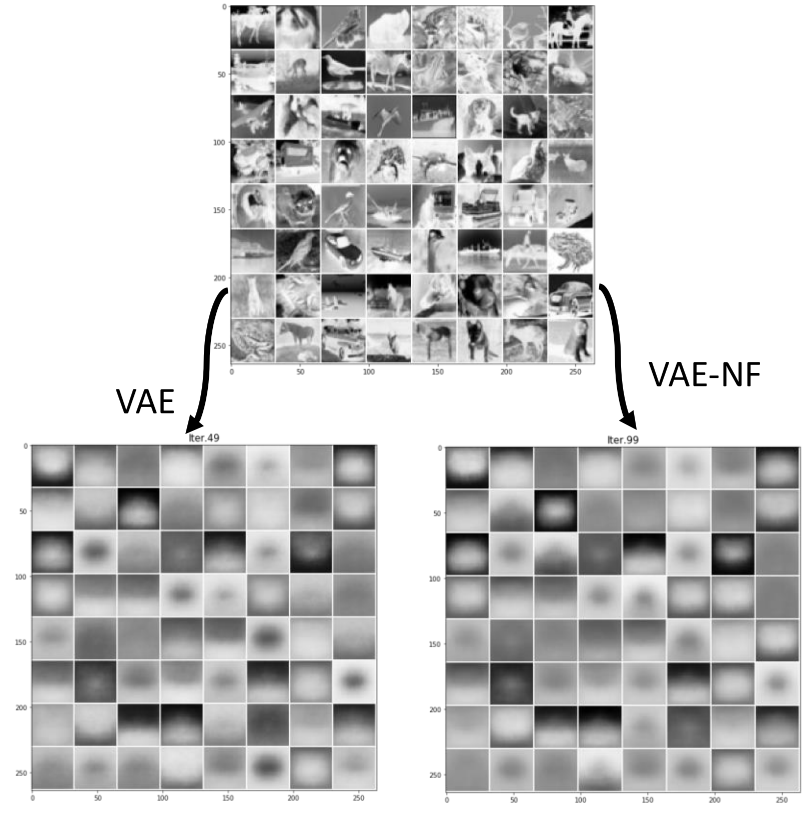


MNIST

Normalizing Flows with VAE (Additional Datasets)



F-MNIST



CIFAR-10

Blurry images from VAE:

- Using Convolution and Transpose convolution in encoder and decoder respectively might help
- CIFAR-10 trained for 100 epochs only.

Summary

- Normalizing flows (NF) were originally proposed to overcome the simplifying assumption of normally distributed posterior distributions in variational autoencoders (VAE).
- In this work, I tried to compare the performance of vanilla VAE with VAE using NFs.
- As observed in the results on MNIST, and FMNIST, the addition of Normalizing flows does not offer apparent improvements in reconstruction or generation. However it must be noted that Normalizing flows uses a planar flow model. Using a more complex flow might help the VAE.
- The reconstructed and generated images are blurry. When compared to other methods like GANs it is pointed out that the expectation operator in the ELBO loss might be the cause for this. However it is an open area of research and an area for future works.

References:

- Implementation for this work (final update soon): https://github.com/shams-sam/EE695-ILGM.
- Kalman and Bayesian Filters in Python: https://github.com/rlabbe/Kalman-and-Bayesian-Filters-in-Python is a good resource for introduction to other filtering approaches.
- Franchi, Gianni, et al. "TRADI: Tracking deep neural network weight distributions." *European Conference on Computer Vision (ECCV) 2020*. (code for this paper is not released; vectorized implementation is available in my project: https://github.com/shams-sam/EE695-ILGM).
- Kingma, Diederik P., and Max Welling. "Auto-encoding variational bayes." *arXiv preprint arXiv:1312.6114* (2013).
- Kobyzev, Ivan, Simon Prince, and Marcus Brubaker. "Normalizing flows: An introduction and review of current methods." *IEEE Transactions on Pattern Analysis and Machine Intelligence* (2020).