

XAI: Cluster Variational Inference Notes

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Abstract

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1 Workflow

Variational Inference model explanation

The purpose of this report is to introduce the Variational Inference Cluster algorithm and experiment with it.

Situations:

1. ML model interpretability is attracting more attention in order to improve model performance and robustness in industrial applications.
2. Briefly outline the importance of machine learning interpretability in the medical field, financial field, and autonomous driving. Explainable AI and adversarial attacks highlight the importance of understanding models.
3. Explainable AI (XAI) aims to understand the model's decision-making process.
4. Adversarial attacks exploit key features to influence the output.

Problem:

1. Applying the model in the wrong field.
2. The model outputs something incorrect, and people are not able to understand why.
3. Users blindly trust the model.
4. Do XAI and adversarial attack techniques share the same results?

Solution:

1. Examine and compare state-of-the-art techniques.
2. Use Variational Inference for model explanation.

Evaluation:

Show the comparison of results.

2 Introduction

Machine learning encompasses a variety of tasks, including classification, segmentation, and modern techniques such as generative models. One fundamental aspect of machine learning is classification, which involves categorizing data into labeled and unlabeled datasets. This process includes techniques from both supervised and unsupervised learning. A key feature

of unsupervised learning is clustering, an algorithm designed to group data into distinct clusters based on inherent similarities. Clustering is an unsupervised learning technique aimed at partitioning data into different clusters. One of the significant challenges in this field is the difficulty in understanding how models work analytically, which can lead to unpredictable results in critical applications such as medical diagnosis, financial fraud detection, and autonomous driving. Therefore, understanding model interpretability for key features is crucial. This is where the concept of explainable AI (XAI) becomes relevant. XAI is a subfield of artificial intelligence focused on making AI models more transparent and understandable to humans.

Another important area of research is adversarial attacks, which further underscores the importance of XAI and the need to comprehend model behavior. While XAI aims to elucidate the model's decision-making process, adversarial attacks seek to exploit the model's vulnerabilities.[1] [2] The robustness of models is crucial for their real-world applications, and understanding the dynamics between XAI and adversarial attacks is essential for improving model interpretability and reliability. Despite their differences, both fields highlight the necessity of understanding AI models.

In this paper, we explore state-of-the-art techniques in explainable AI (XAI) and adversarial attacks, focusing on how they interpret features in images differently. Through our exploration, we found that images in high-dimensional spaces significantly contribute to model complexity. This complexity aligns with the challenges posed by both XAI and adversarial attacks. Specifically, while XAI aims to elucidate the decision-making process of complex models, adversarial attacks exploit the vulnerabilities inherent in these high-dimensional representations. Understanding these dynamics is crucial for improving model robustness and interpretability. As we advocate for the idea of XAI, we introduce the Variational Inference Clustering algorithm and experiment with it. This algorithm is a popular XAI method used to interpret features in images.

3 Related Work

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In this paper, we explore state-of-the-art XAI and adversarial attack techniques and how they interpret features in images differently. From the foundations of machine learning and deep learning, we know that improved predictive accuracy often comes with increased model complexity. This complexity can decrease the in-sample error (E_{in}) but may increase the out-of-sample error (E_{out}) [3, 4, 5]. To better understand models, it is essential to interfere with their decision-making processes.

The GradCAM[6], algorithm is a popular XAI algorithm.

4 Experiments

... VI Structures:

The variational inference algorithm is a popular XAI method used to interpret features in images. The clusters example[7]

Formulation:

$$\begin{aligned}
z_j &\sim \mathcal{N}(m^2, s^2) \text{ for } j = 1, \dots, K \\
c_i &\sim \mathcal{U}(K) \text{ for } i = 1, \dots, N \\
x_i &\sim \mathcal{N}(c_i^T \mu, 1) \text{ for } i = 1, \dots, N \\
y &\sim CNN
\end{aligned} \tag{1}$$

ELBO function:

$$ELBO = E_q[\log p(x, \hat{z})] - E_q[\log q(\hat{z})] \tag{2}$$

$$= E_q[\log p(x, z, c, y) - \log q(z, c, y)] \tag{3}$$

Encoder $q(\cdot)$:

$$\begin{aligned}
\log q(z, c, y) &= \log [q(z|m, s^2) q(c|\phi) q(y|z, c)] \\
&= \log \left[\prod_j q(z_j|m_j, s_j^2) \prod_i q(c_i|\phi_i) q(y|z, c) \right] \\
&= \sum_j \log q(z_j|m_j, s_j^2) + \sum_j \log \phi_j + \log \text{pred}_y \\
&\propto \sum_j \frac{-1}{2} \left(\log s^2 + \frac{(z_j - m_j)^2}{s_j^2} \right) + \sum_j \log \phi_j + \log \text{pred}_y
\end{aligned} \tag{4}$$

Decoder $p(\cdot)$:

$$p(c_i) = \frac{1}{K}$$

$$p(y) = N(y|0, 1)$$

$$\begin{aligned}
\log p(x_i \mid c_i, z_j, y) &= \log \prod_j p(x_i \mid z_j, y)^{c_{ij}} \prod_j p(c, z|y) p(y) \\
&\propto \sum_j c_j \log p(x_i \mid z_j) - \sum_j c_j \log \left(-\frac{1}{2\pi} e^{-\frac{1}{2} \left(\frac{z_j - \mu_y}{1} \right)^2} \right) \\
&\propto \sum_j c_j \log p(x_i \mid z_j) - \frac{1}{2} \sum_j c_j \left(\frac{z_j - \mu_y}{1} \right)^2 \\
&\propto -\frac{1}{2} \left(\sum_j c_j \left(\frac{x_i - m_j}{1} \right)^2 + \sum_j c_j \left(\frac{z_j - \mu_y}{1} \right)^2 \right)
\end{aligned}$$

$$ELBO = E_q[\log p(x, z, c, y) - \log q(z, c, y)]$$

$$= E_q[-\frac{1}{2}(\sum_j c_j (x_i - m_j)^2 + \sum_j c_j (z_j - \mu_y)^2) + \frac{1}{2} \left(\sum_j \log s^2 \right) - \sum_j \log \phi_j - \log \text{pred}_y]$$

4.1 Full Connected Variational Inference

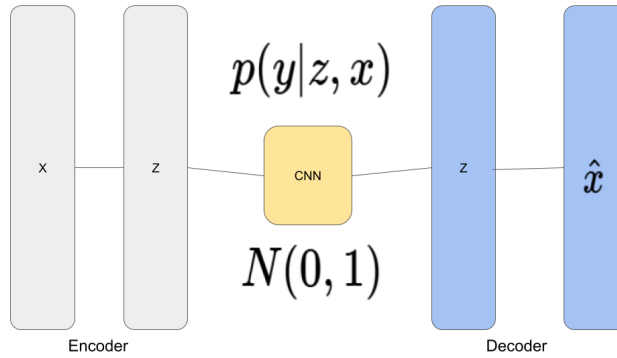


Figure 1: Using 784 $z = \{\mu, s\}$

Code 1: Full connected VI loss function

```

1 def loss_elbo(x, mu, log_var, phi, x_recon, model, predicted):
2     # HACK: use the CNN model prediction as the input
3     t1 = 0.5 * (mu.view(1, -1) - mu_y.view(-1, 1)) ** 2
4     t1 = phi * t1
5     t1 = -t1.mean()
6
7     # NOTE: Alternative implementation

```

```

8     t2 = 0.5 * (x - x_recon) ** 2
9     t2 = phi * t2
10    t2 = torch.mean(t2)
11
12    t3 = 0.5 * log_var.exp().mean()
13
14    t4 = -torch.log(phi + 1e-10).mean()
15
16    # HACK: use the CNN model prediction as the input
17    model.eval()
18    input = x_recon.view(1, 1, 28, 28)
19    # Forward pass
20    outputs = model(input)
21    outputs = F.softmax(outputs, dim=1)
22    outputs = torch.clamp(outputs, 1e-10, 1 - 1e-10)
23    t5 = -torch.log(outputs[:, predicted])
24    return -(t1 + t2 + t3 + t4 + t5) + lamb

```

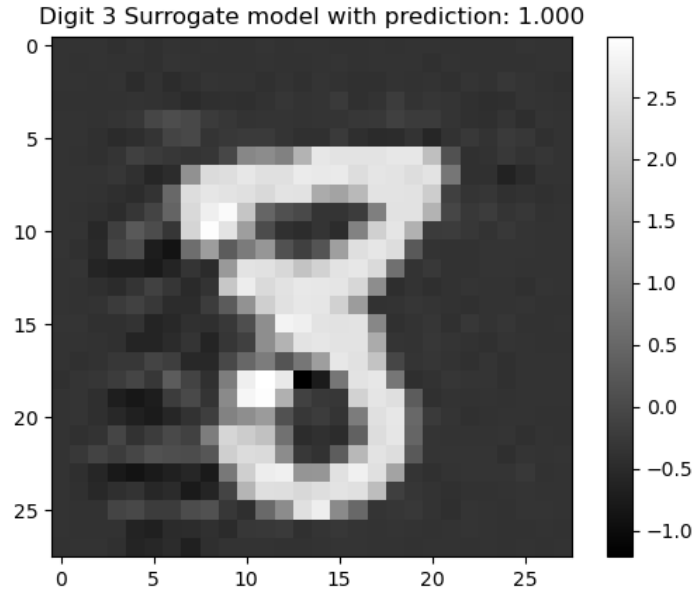


Figure 2: MNIST Prediction with 784 $z = \{\mu, s\}$

4.2 Conv2d Variational Inference

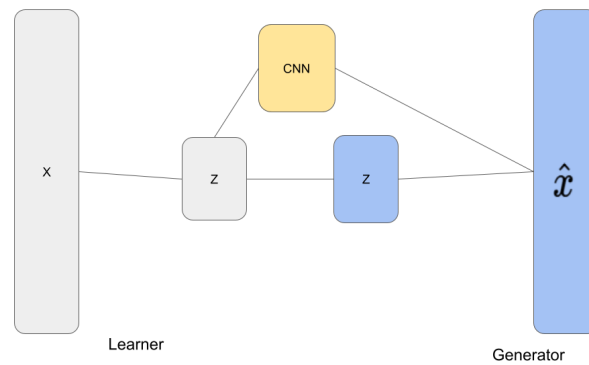


Figure 3: Using GAN and VAE method with conv2d

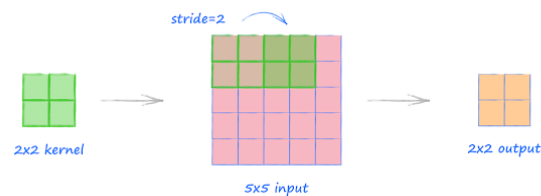


Figure 4: use conv2d kernel size 2x2 and stride 2

Code 2: GAN and VAE model

```

1  class generator(nn.Module):
2      def __init__(self, channels_img):
3          super().__init__()
4          self.channels_img = channels_img
5          # self.features_d = features_d
6          self.k = 2
7          # decoder
8          self.decoder = nn.Sequential(
9              # NOTE: convTranspose2d output = (input -1)*s -2p + k + op
10             # (14-1)*2 + 2 = img 28x28
11             nn.ConvTranspose2d(
12                 channels_img, channels_img, kernel_size=2, stride=2,
13                 padding=0
14             ),
15             nn.Tanh(),
16         )
17
18         self.p_layer = nn.Sequential(
19             # NOTE: convTranspose2d output = (input -1)*s -2p + k + op
20             # (14-1)*2 + 2 = img 28x28
21             nn.ConvTranspose2d(
22                 channels_img, channels_img * self.k, kernel_size=2,
23                 stride=2, padding=0
24             ),
25             nn.Tanh(),
26         )

```

```

24         )
25
26     def forward(self, x, z):
27         p = self.p_layer(z)
28         p = F.softmax(p, dim=0)
29         # x_recon = self.decoder(z) * p[:, 0, :, :] + x * (p[:, 1, :,
30             :])
31         x_recon = self.decoder(z)
32         return x_recon, p
33
34 class learner(nn.Module):
35     def __init__(self, channels_img):
36         super().__init__()
37         self.channels_img = channels_img
38         # self.features_d = features_d
39         self.k = 2
40         # encoder
41         # latent mean and variance
42         self.mean_layer = nn.Sequential(
43             # NOTE: conv2d output = (input + 2p -k)/s +1
44             # (28-2)/2 +1 = img 14x14
45             nn.Conv2d(channels_img, channels_img, kernel_size=2,
46                 stride=2),
47             nn.InstanceNorm2d(channels_img, affine=True),
48             nn.LeakyReLU(0.2),
49         ) # latent mean and variance
50         self.logvar_layer = nn.Sequential(
51             # NOTE: conv2d output = (input + 2p -k)/s +1
52             # (28-2)/2 +1 = img 14x14
53             nn.Conv2d(channels_img, channels_img, kernel_size=2,
54                 stride=2),
55             nn.InstanceNorm2d(channels_img, affine=True),
56             nn.LeakyReLU(0.2),
57         )
58
59     def reparameterization(self, mean, var):
60         # mean = mean.view(mean.size[0], -1)
61         # var = var.view(var.size[0], -1)
62         epsilon = torch.randn_like(var).to(device)
63         z = mean + var * epsilon
64         return z
65
66     def encode(self, x):
67         mean, logvar = self.mean_layer(x), self.logvar_layer(x)
68         return mean, logvar
69
70     def forward(self, x):
71         mean, log_var = self.encode(x)
72         z = self.reparameterization(mean, log_var)
73         return z, mean, log_var

```

Code 3: GAN and VAE loss function

```

1 epochs = 1000
2 leaner_epochs = 10
3 predicted = true_y
4 # predicted = 9
5 G = generator(1).to(device)
6 L = learner(1).to(device)
7
8 opt_G = torch.optim.Adam(G.parameters(), lr=0.005)
9 opt_L = torch.optim.Adam(L.parameters(), lr=0.005)
10
11
12 def loss_function(x, x_recon, mean, log_var, p):
13     alpha = torch.sum(p[:, 0, :, :])
14     # reproduction_loss = F.mse_loss(x_recon * p[:, 0, :, :], x * p[:,
15     #                                0, :, :])
16     reproduction_loss = F.mse_loss(x_recon, x)
17     KLD = -0.5 * torch.sum(1 + log_var - mean.pow(2) - log_var.exp())
18
19     return reproduction_loss + KLD
20
21 # %%
22
23 for epoch in range(epochs + 1):
24     for leaner_epoch in range(leaner_epochs + 1):
25         opt_L.zero_grad()
26         x = img.clone().to(device)
27         x = x.view(1, 1, 28, 28)
28         z, mean, log_var = L(x)
29         x_recon, p = G(x, z)
30         # Get the index of the max log-probability
31         model.eval()
32         critic_fake = F.softmax(model(x_recon), dim=1)[0][predicted]
33
34         loss_L = -(torch.mean(critic_fake))
35         # loss = loss_function(x, x_recon, mean, log_var) - torch.log(
36         #     critic_real + 1e-5) * (
37         #         -torch.log(critic_fake + 1e-5)
38         # )
39
40         loss_L.backward(retain_graph=True)
41         opt_L.step()
42
43     opt_G.zero_grad()
44     x = img.clone().to(device)
45     x = x.view(1, 1, 28, 28)
46     z, mean, log_var = L(x)
47     x_recon, p = G(x, z)
48
49     model.eval()
50     critic_fake = F.softmax(model(x_recon), dim=1)[0][predicted]
51     t1 = -torch.sum(torch.log(critic_fake + 1e-5))
52     t2 = loss_function(x, x_recon, mean, log_var, p)

```



```
52
53     # NOTE: original loss function
54     loss_G = t1 + t2
55     # NOTE: alternative loss function, from GAN
56     # loss_G = torch.mean(critic_fake)
57
58     loss_G.backward()
59     opt_G.step()
```

Table 1: Experiments Comparison table with top n-th variance(v3)

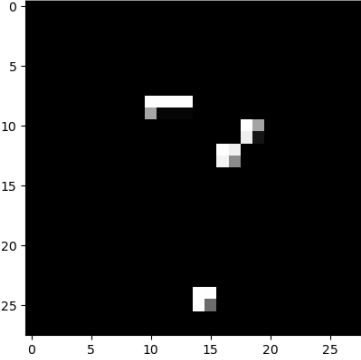
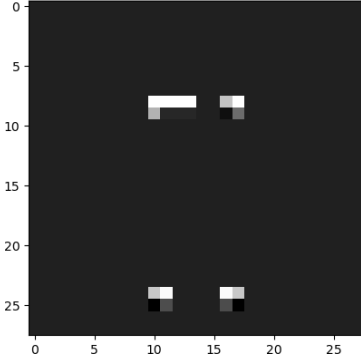
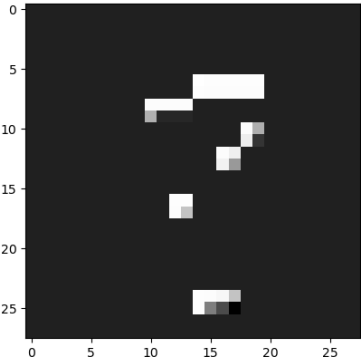
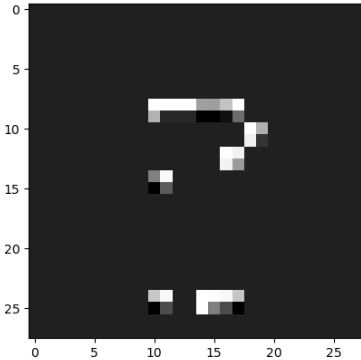
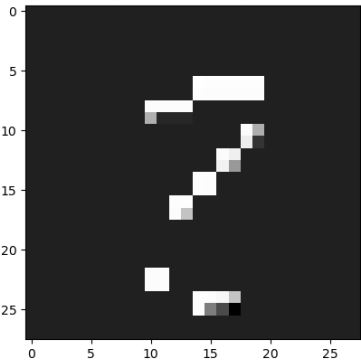
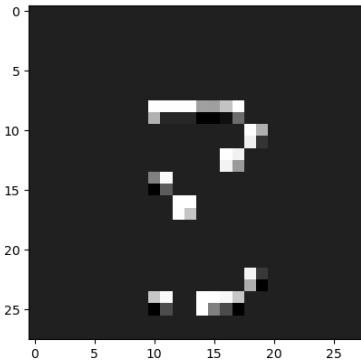
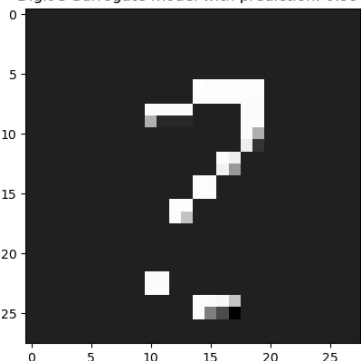
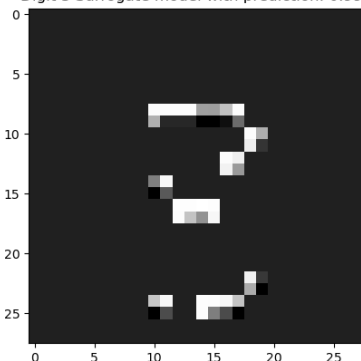
<p>$n = 5$</p> <p>Digit 3 Surrogate model with prediction: 0.666</p> 	<p>$n = 5$</p> <p>Digit 3 Surrogate model with prediction: 0.646</p> 
<p>$n = 10$</p> <p>Digit 3 Surrogate model with prediction: 0.866</p> 	<p>$n = 10$</p> <p>Digit 3 Surrogate model with prediction: 0.981</p> 
<p>$n = 12$</p> <p>Digit 3 Surrogate model with prediction: 0.953</p> 	<p>$n = 12$</p> <p>Digit 3 Surrogate model with prediction: 0.997</p> 
<p>$n = 13$</p> <p>Digit 3 Surrogate model with prediction: 0.994</p> 	<p>$n = 13$</p> <p>Digit 3 Surrogate model with prediction: 0.995</p> 

Table 2: Experiments Comparison table with top n-th variance(v3)

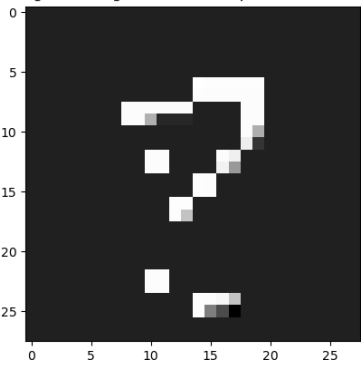
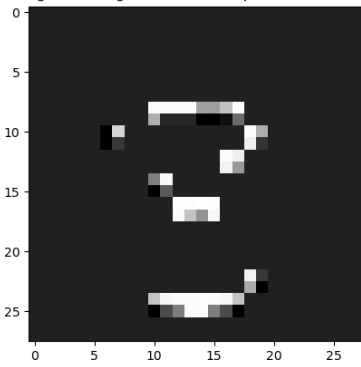
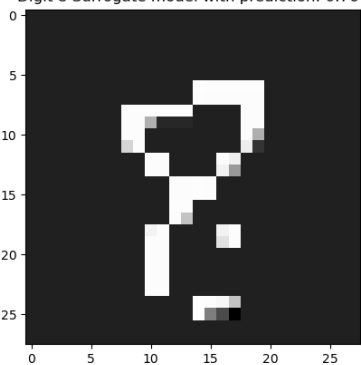
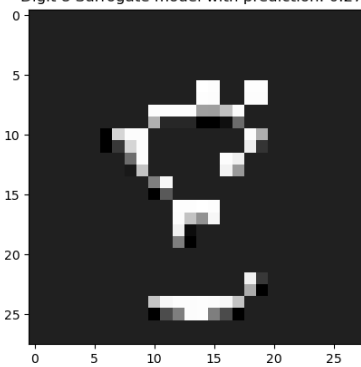
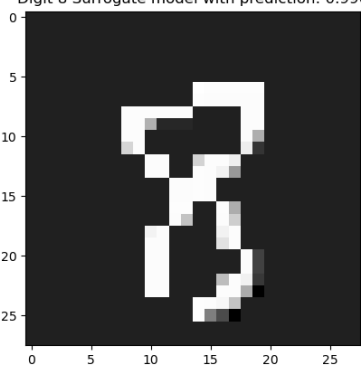
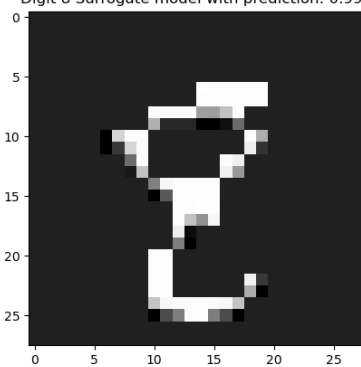

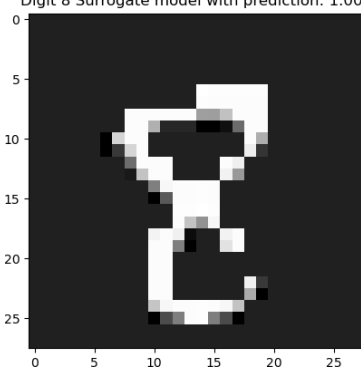
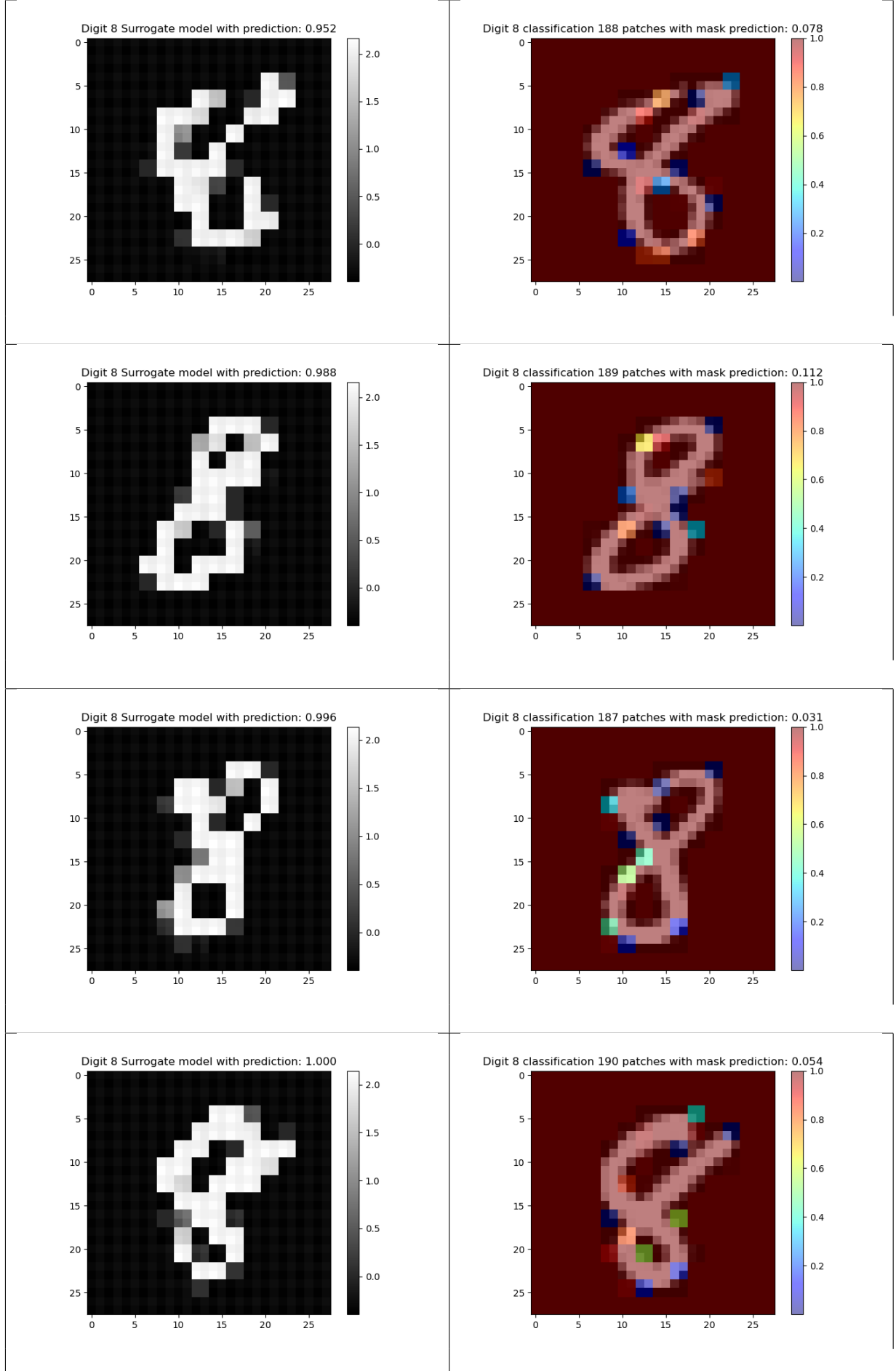
<p>$n = 15$</p> <p>Digit 3 Surrogate model with prediction: 0.998</p> 	<p>$n = 15$</p> <p>Digit 3 Surrogate model with prediction: 0.996</p> 
<p>$n = 20$</p> <p>Digit 8 Surrogate model with prediction: 0.764</p> 	<p>$n = 20$</p> <p>Digit 8 Surrogate model with prediction: 0.278</p> 
<p>$n = 25$</p> <p>Digit 8 Surrogate model with prediction: 0.990</p> 	<p>$n = 25$</p> <p>Digit 8 Surrogate model with prediction: 0.998</p> 
<p>$n = 30$</p> <p>Digit 8 Surrogate model with prediction: 1.000</p> 	<p>$n = 30$</p> <p>Digit 8 Surrogate model with prediction: 1.000</p> 

Table 3: Train one class Experiments Comparison table with mask $C < 0.1$ (v4)



5 Experiment Results 2.0

Formulation (Equation ideal Similar to [7]) Structure (Concept similar to [8]):

$$z_j \sim \mathcal{N}(\mu, \sigma^2) \text{ for } j = 1, \dots, K$$

$$c_i \sim \phi(K) \text{ for } i = 1, \dots, N$$

$$x_i \sim \mathcal{N}(c_i^T z, 1) \text{ for } i = 1, \dots, N$$

$$y \sim CNN$$

(5)

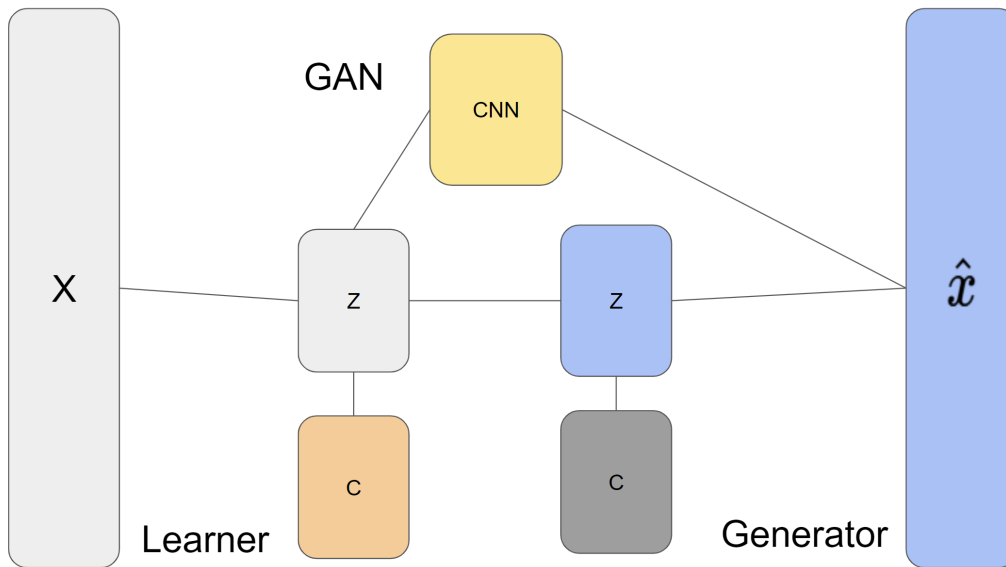


Figure 5: Using GAN and VAE method with conv2d

The goal is to minimize the loss function:

$$\underbrace{\arg \max}_{ELBO} \underbrace{\arg \max}_z \mathbb{E}_{z \sim p_z(z)}[L(z)] + ELBO$$

$$ELBO = E_q[\log p(x, z, c, y) - \log q(z, c, y)]$$

$$= E_q[-\frac{1}{2}(\sum_j c_j (x_i - m_j)^2 + \sum_j c_j (z_j - \mu_y)^2) + \frac{1}{2} \left(\sum_j \log s^2 \right) - \sum_j \log \phi_j - \log \text{pred}_y]$$

In my experiments, $k = 10$, Some issues with the model:

1. Mode collapse: The model is not able to generate diverse samples.
Remedy: add regularization term to the model[9].

$$\lambda \int q(z) \|G(z) - G^o(z)\|^2 dz$$

Where $G^o(z)$ is the previous data distribution.

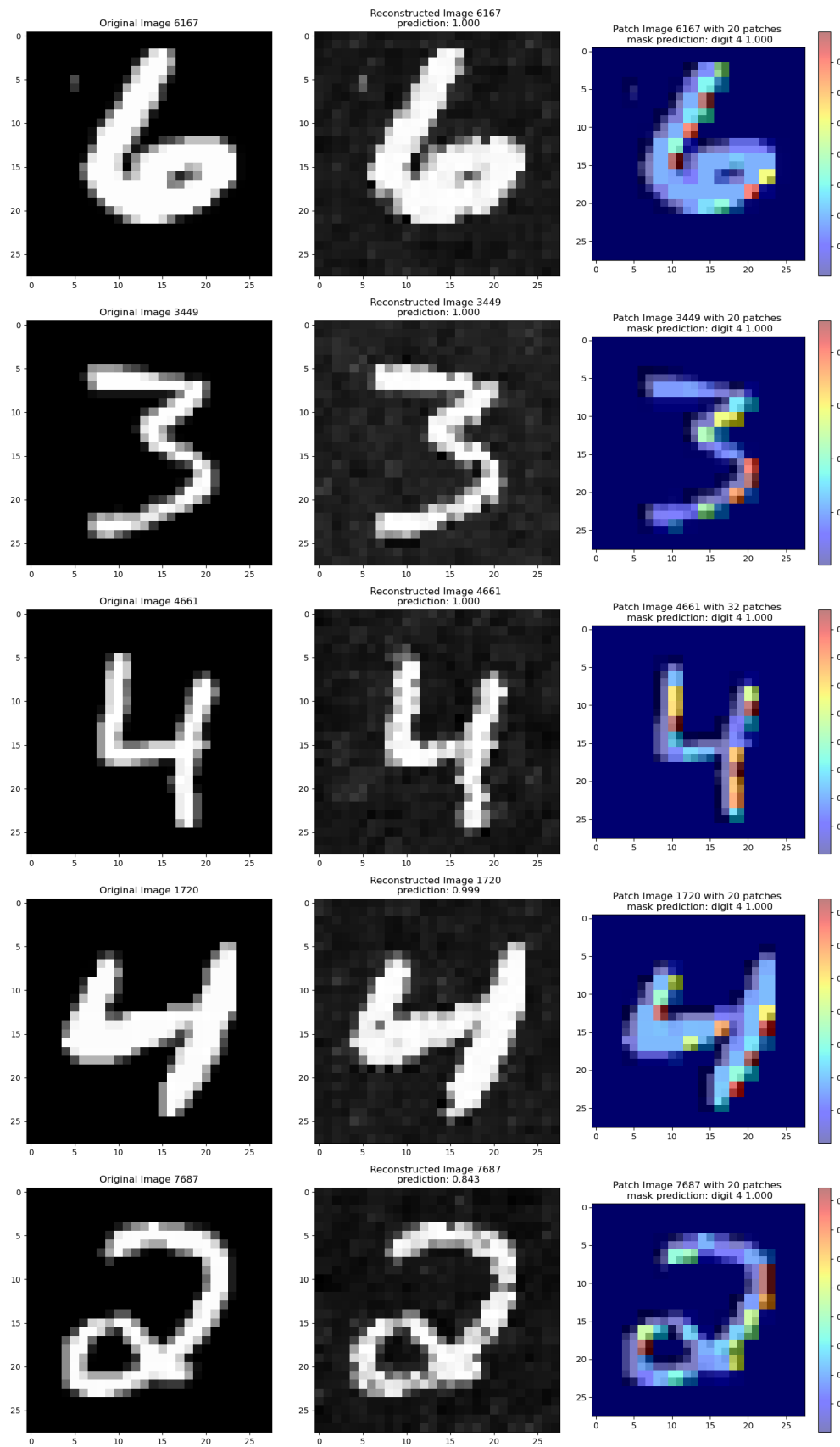


Figure 6: Conv2d output: mode collapse

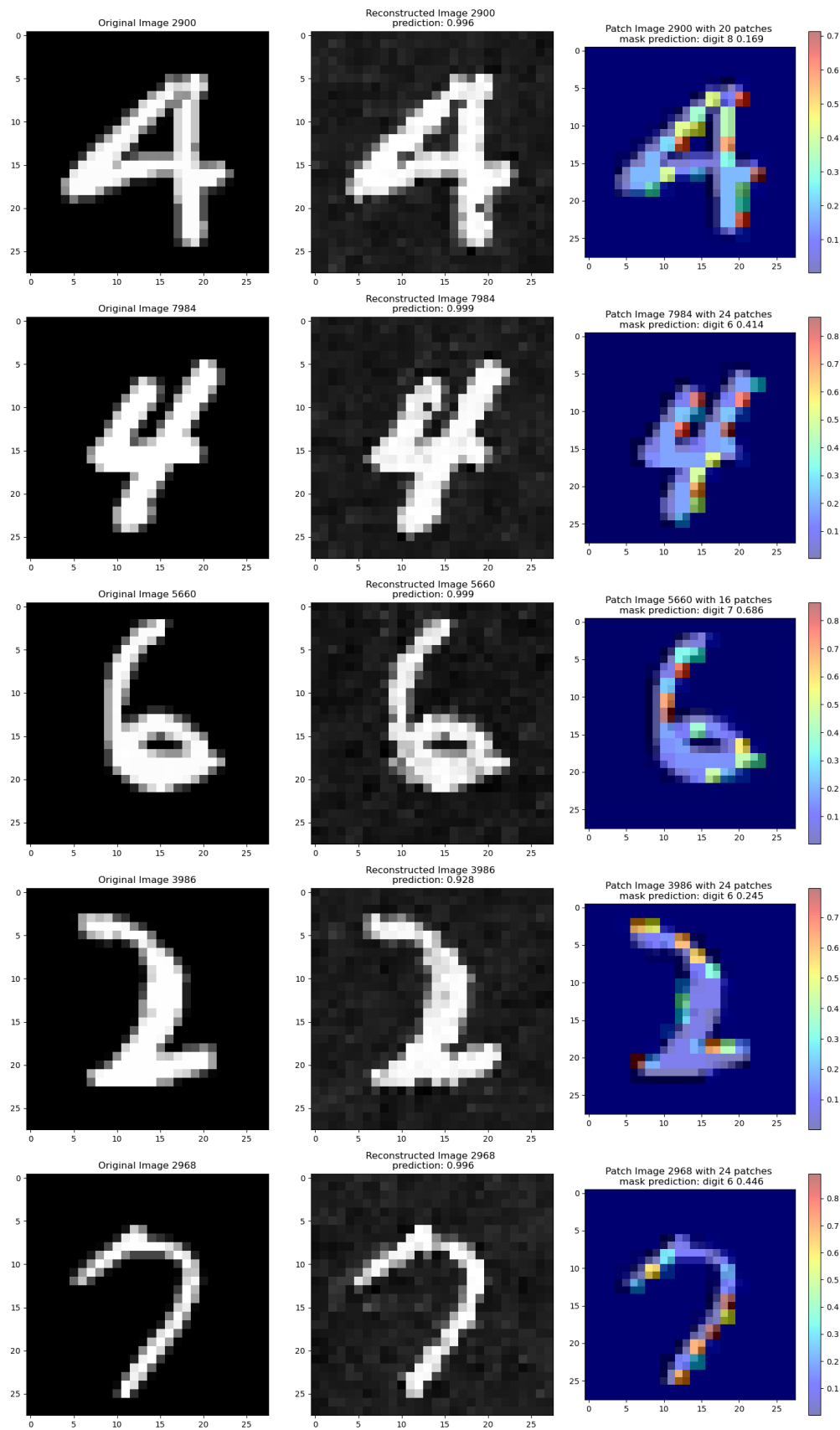


Figure 7: Conv2d output 1

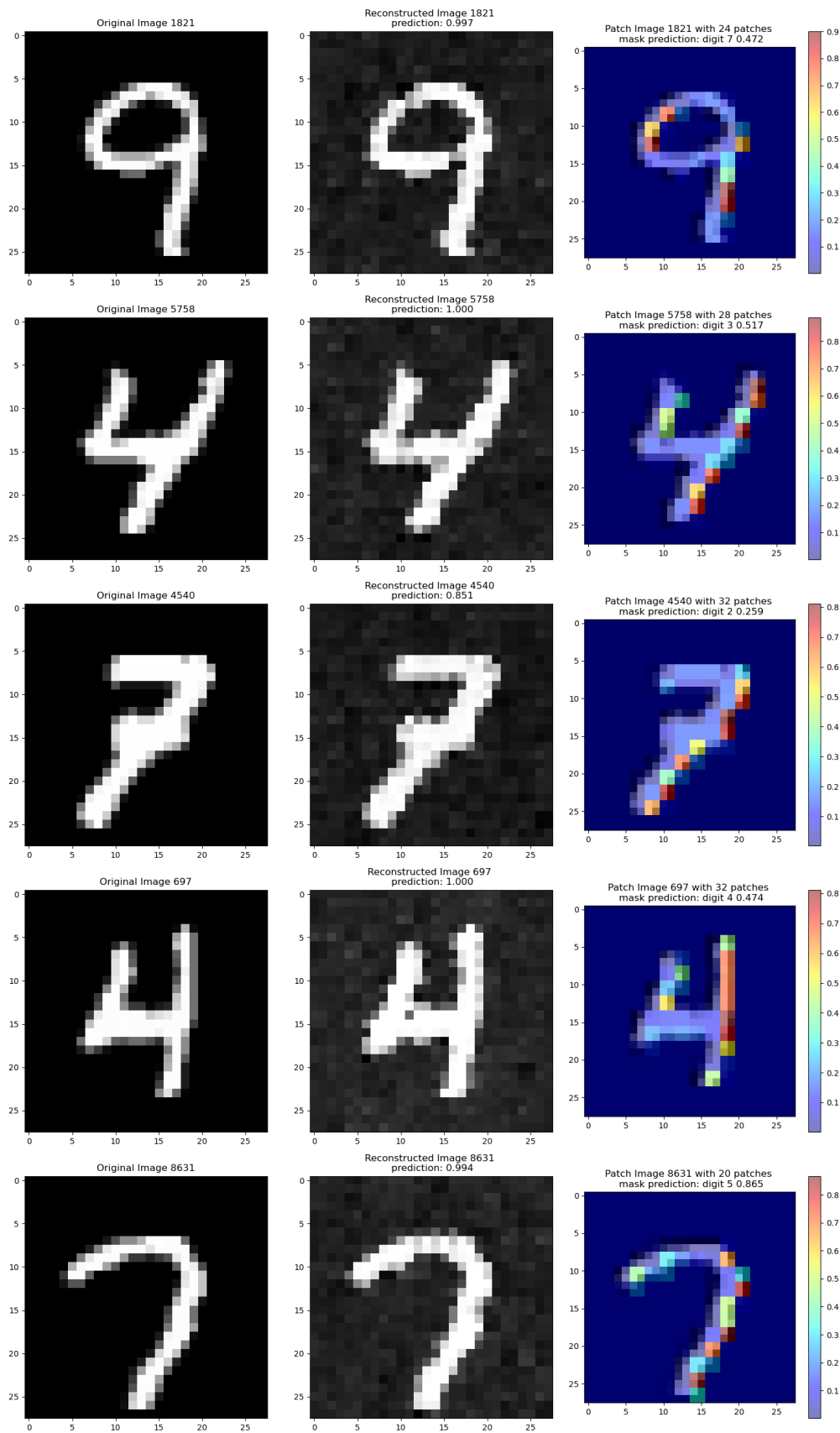


Figure 8: Conv2d output 2

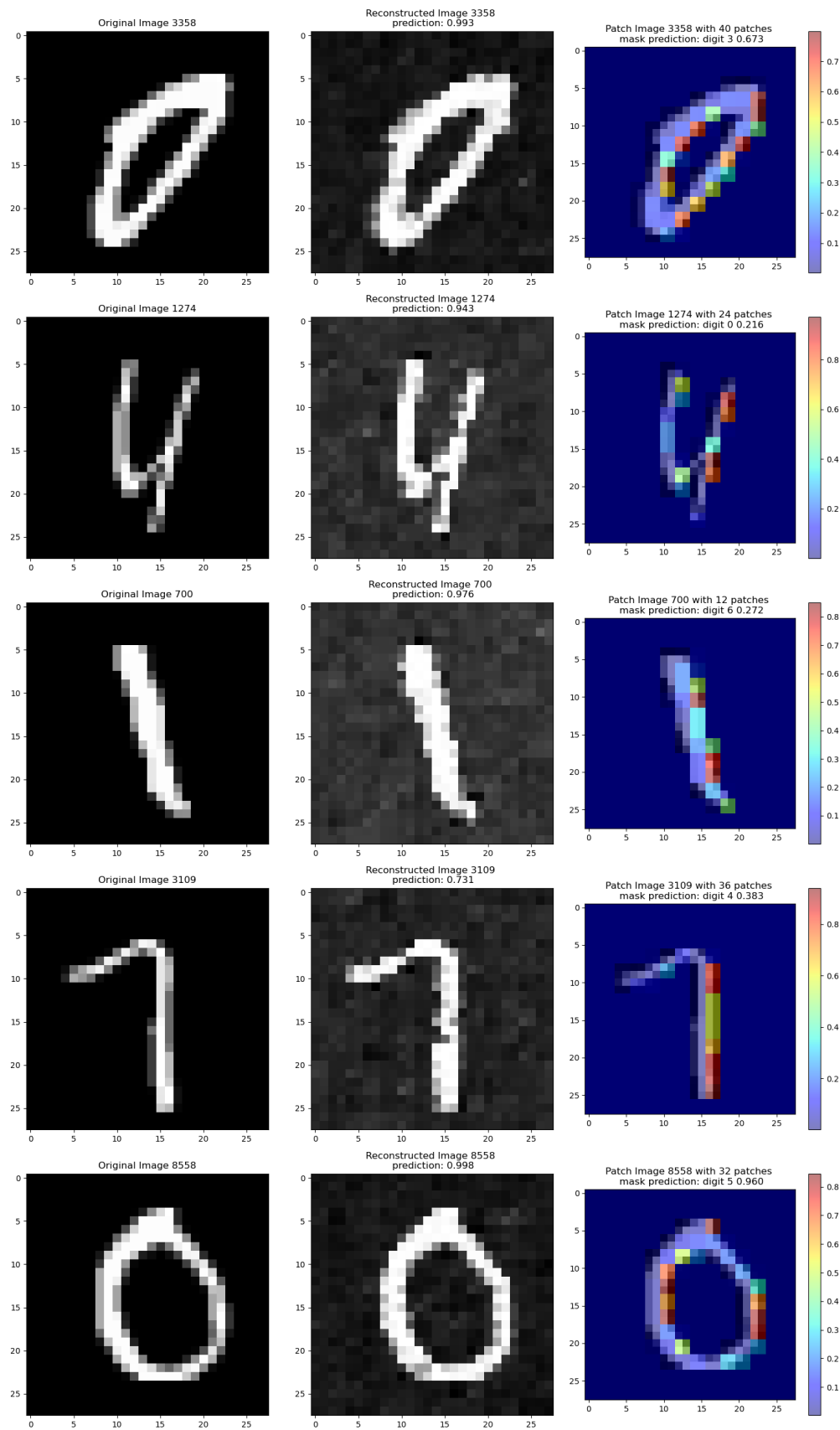


Figure 9: Conv2d output 3

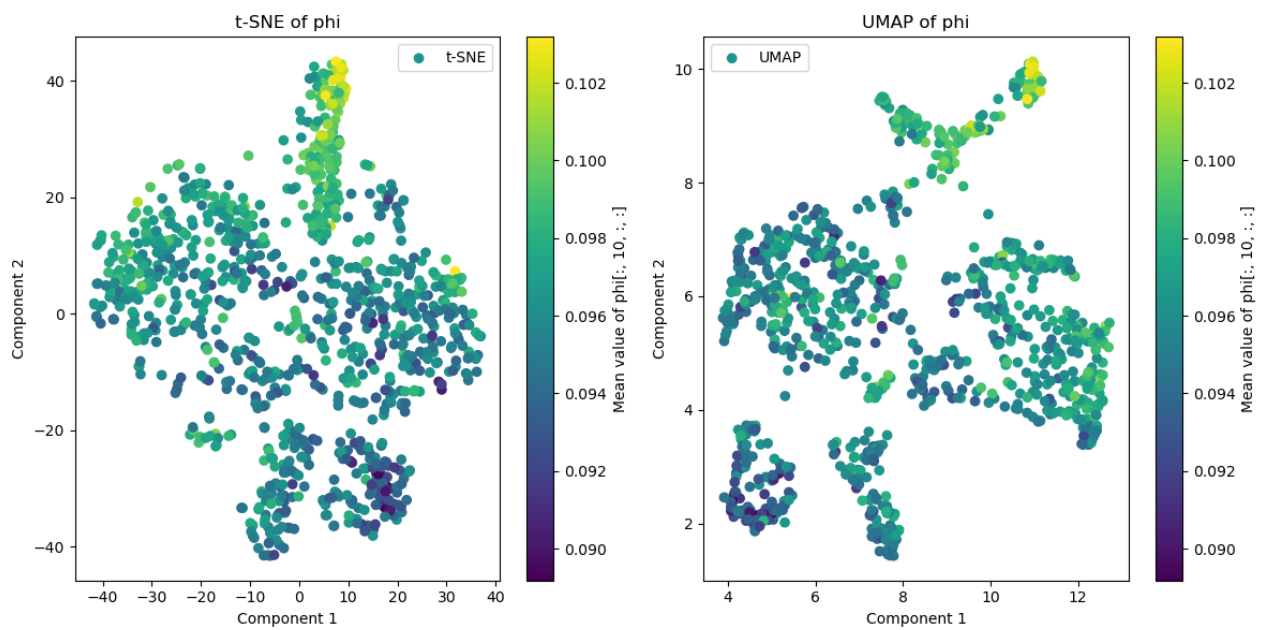


Figure 10: T-SNE vs UMAP

6 Future Work

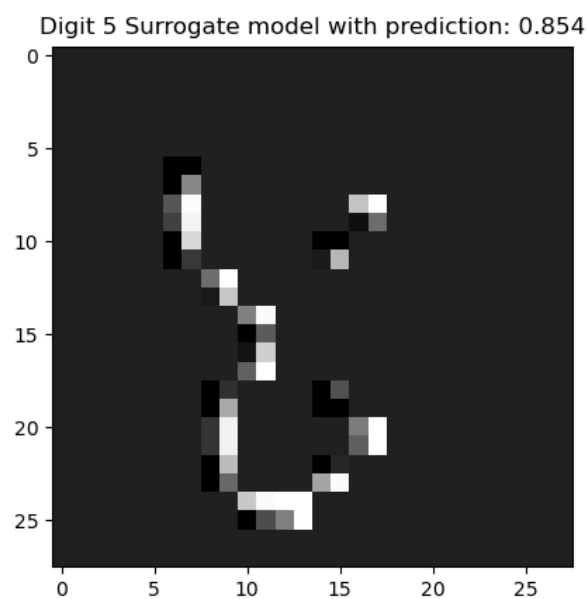
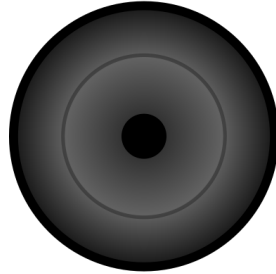


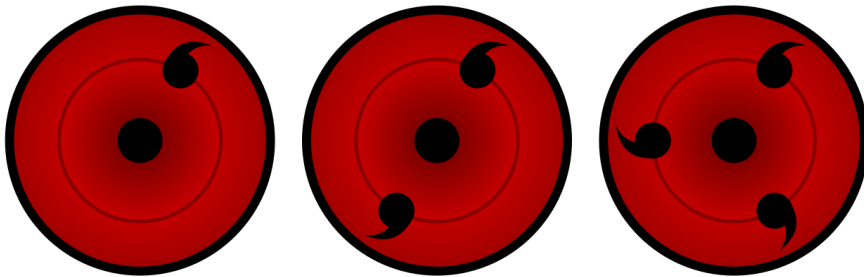
Figure 11: Using conv2d and GAN

Sharingan Evolution:

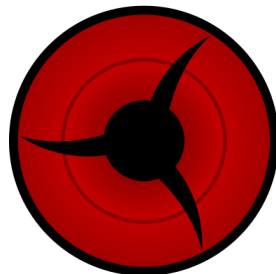
Sharingan evolution



Inactive sharingan



Classics sharingan with one, two and three tomoe



Proto-mangekyō sharingan

Figure 12: Sharingan

7 Conclusion

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References

- [1] A. Athalye, L. Engstrom, A. Ilyas, and K. Kwok, “Synthesizing Robust Adversarial Examples,” June 2018.
- [2] S.-M. Moosavi-Dezfooli, A. Fawzi, O. Fawzi, and P. Frossard, “Universal adversarial perturbations,” Mar. 2017.
- [3] S. Shalev-Shwartz and S. Ben-David, *Understanding Machine Learning: From Theory to Algorithms*. New York, NY, USA: Cambridge University Press, 2014.
- [4] L. Devroye, L. Györfi, and G. Lugosi, *A Probabilistic Theory of Pattern Recognition*. New York: Springer, 1996.
- [5] T. Hastie, R. Tibshirani, and J. H. Friedman, *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. Springer Series in Statistics, New York, NY: Springer, second edition, corrected at 12th printing 2017 ed., 2017.
- [6] R. R. Selvaraju, M. Cogswell, A. Das, R. Vedantam, D. Parikh, and D. Batra, “Grad-CAM: Visual Explanations from Deep Networks via Gradient-based Localization,” *International Journal of Computer Vision*, vol. 128, pp. 336–359, Feb. 2020.
- [7] D. M. Blei, A. Kucukelbir, and J. D. McAuliffe, “Variational Inference: A Review for Statisticians,” *Journal of the American Statistical Association*, vol. 112, pp. 859–877, Apr. 2017.
- [8] L. Mescheder, S. Nowozin, and A. Geiger, “Adversarial Variational Bayes: Unifying Variational Autoencoders and Generative Adversarial Networks,”
- [9] J. Su, “Variational Inference: A Unified Framework of Generative Models and Some Revelations,”