

UNCERTAINTY QUANTIFICATION THROUGH METRIC-AWARE SAMPLING USING RIEMANNIAN MANIFOLDS

Trym Hamer Gudvangen

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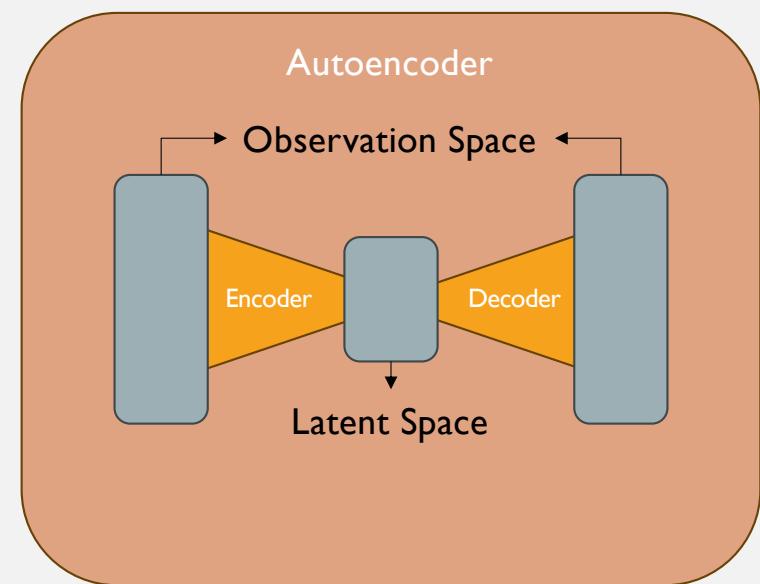
BACKGROUND

VARIATIONAL AUTOENCODER

Goal: Encode data from observation space to a lower dimensional latent distribution and decode latent point to observation space.

How: Special Loss + Reparameterization Trick

Why: Stability, Simplicity, Baseline in differential geometry papers, Probabilistic



VARIATIONAL AUTOENCODER

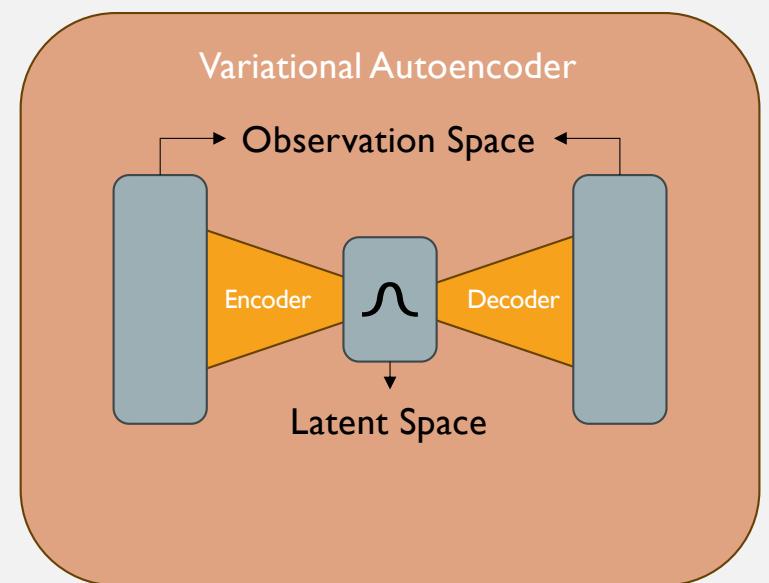
Loss = Evidence Lower Bound = Reconstruction Loss + KL-Divergence

$$L(\phi, \theta; x) = \ln p_\theta(x) - D_{KL}(q_\phi(z|x)||p_\theta(z|x))$$

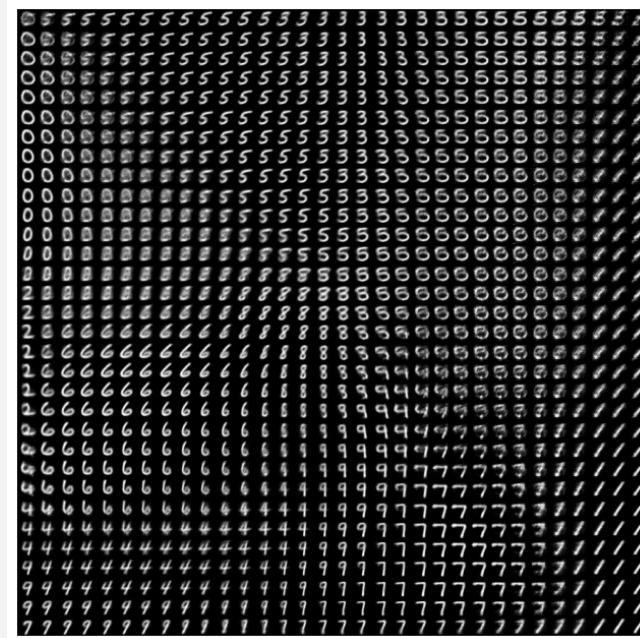
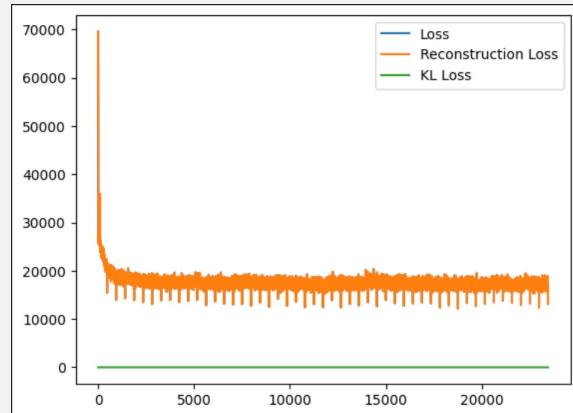
$$\ln p_\theta(x) \geq \mathbb{E}_{z \sim q_\phi(\cdot|x)} \left[\ln \frac{p_\theta(x, z)}{q_\phi(z|x)} \right]$$

Jensen's Inequality

$$\ln p_\theta(x) = \ln \mathbb{E}_{z \sim q_\phi(\cdot|x)} \left[\frac{p_\theta(x, z)}{q_\phi(z|x)} \right] \geq \mathbb{E}_{z \sim q_\phi(\cdot|x)} \left[\ln \frac{p_\theta(x, z)}{q_\phi(z|x)} \right]$$



TRAINING THE VAE



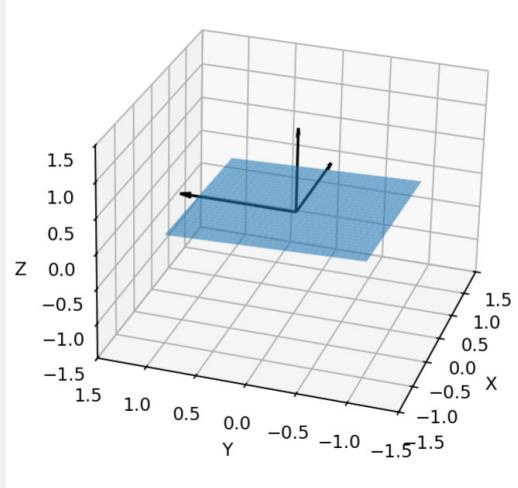
Attempts to make reconstruction better (less blurry)

- Changing activation functions
- Normalization
- BCE instead of MSE for reconstruction loss
- Using Beta VAEs (essentially weighted loss)
- Hierarchy/Depth

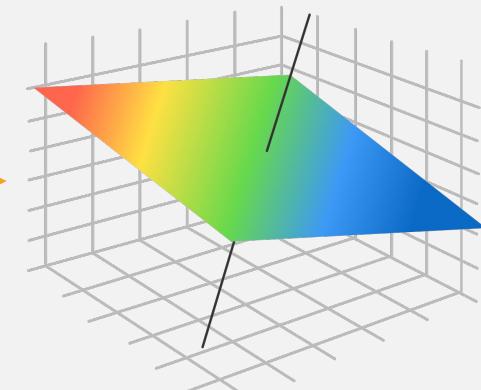
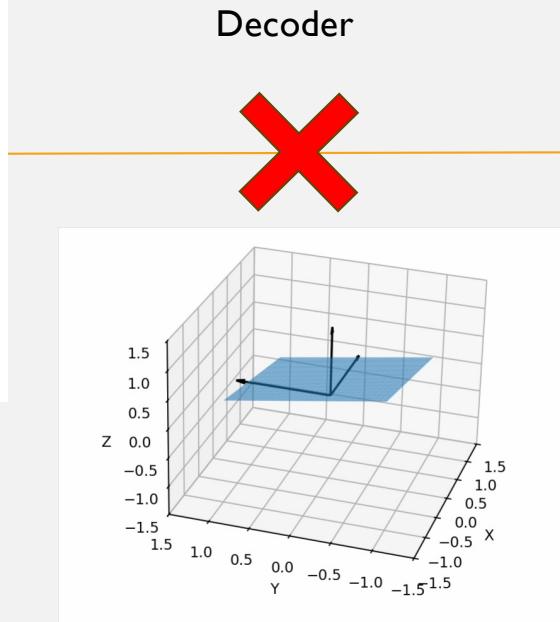
MANIFOLD HYPOTHESIS

- **Assumes:** Real-life high dimensional datasets exist as embedded data manifolds.
- Underlying assumption for generative models
- Important for approach going forward

DIFFERENTIAL GEOMETRY

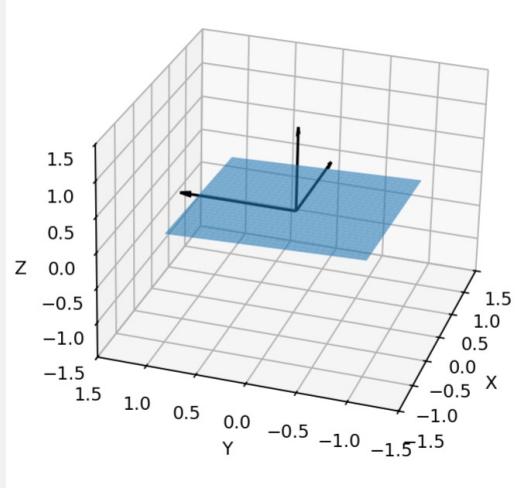


Latent Space (e.g. 2D)
 $\in \mathbb{R}^d$

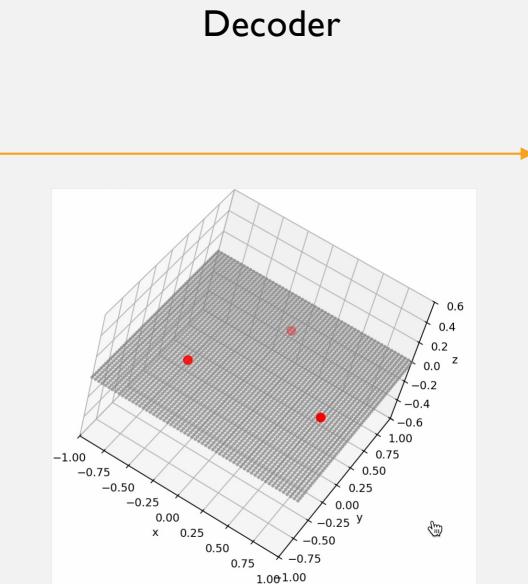


Observation Space (e.g. 3D)
 $\in \mathbb{R}^D$
 $d \ll D$

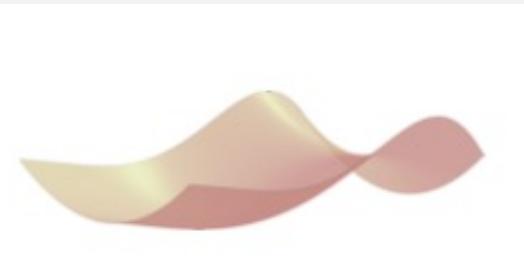
DIFFERENTIAL GEOMETRY



Latent Space (e.g. 2D)
 $\in \mathbb{R}^d$

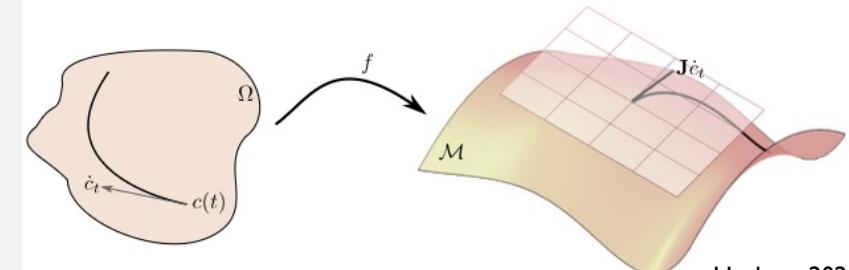


Observation Space (e.g. 3D)
 $\in \mathbb{R}^D$
 $d \ll D$

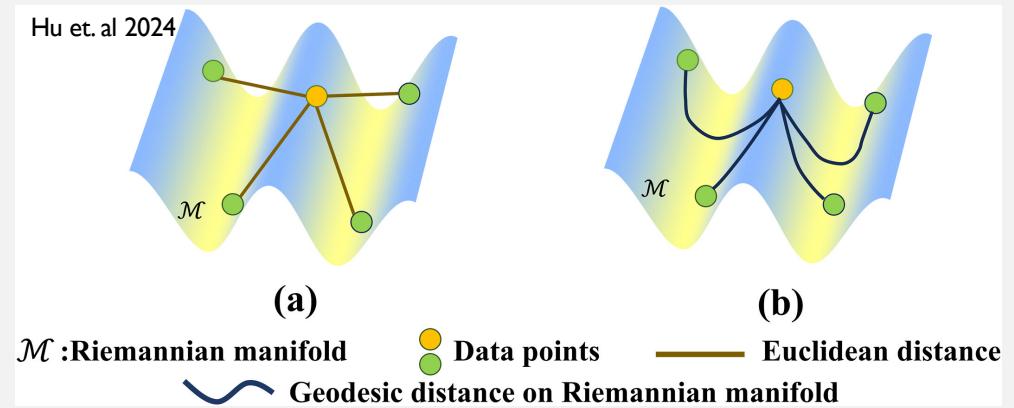


RIEMANNIAN MANIFOLD

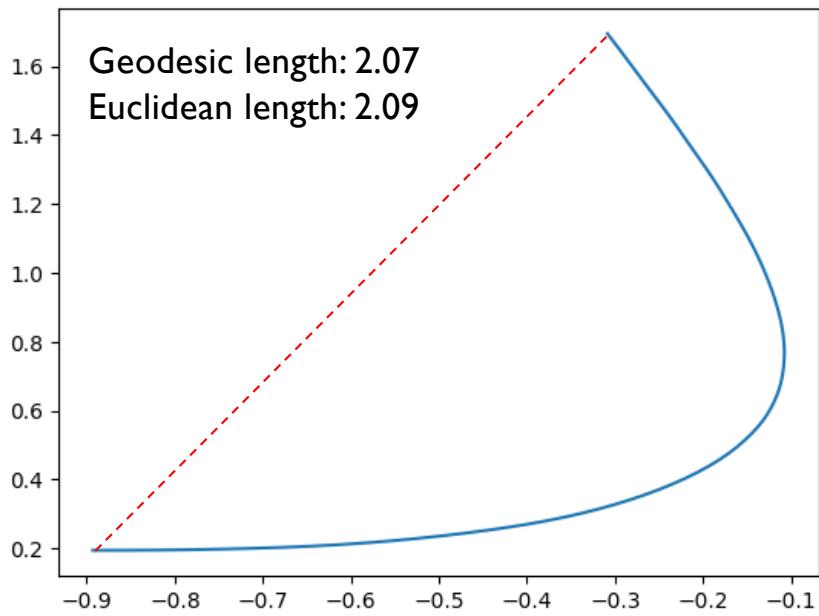
- Curved surface with local Euclidean geometry
- Metrics on Riemannian manifold:
 - Riemannian Metric $M_z = J_z^T J_z$
 - Geodesics
 - Volume Metric $\sqrt{\det(J^T J)}$



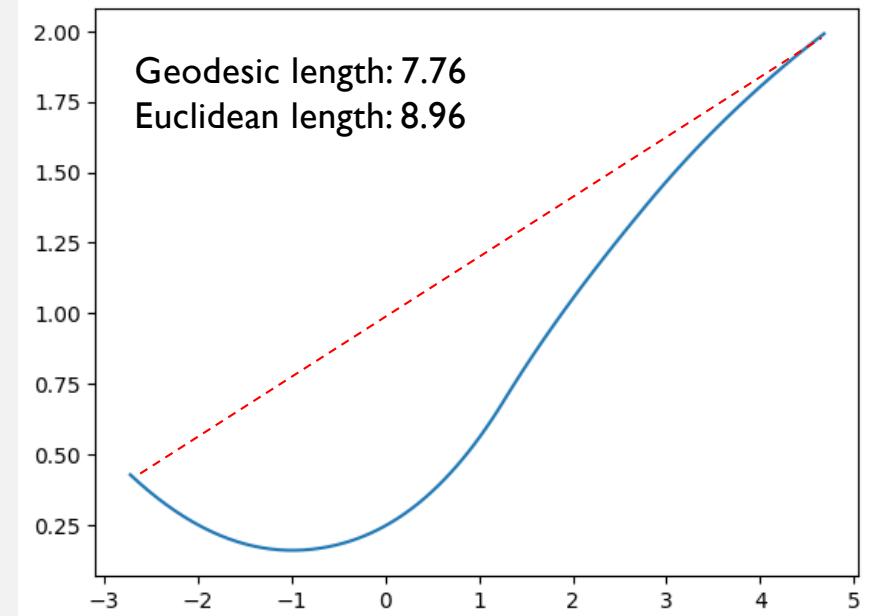
Hauberg 2021



GEODESIC



Two Latent Points from 5-digit inputs

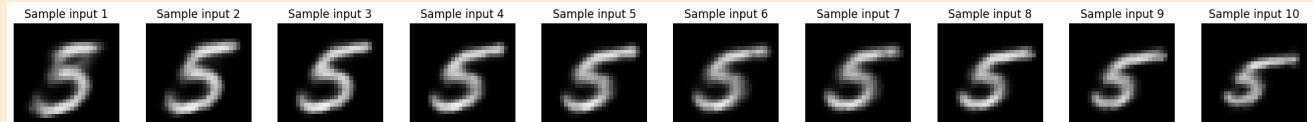


Two Latent Points from 0- and 1-digit inputs

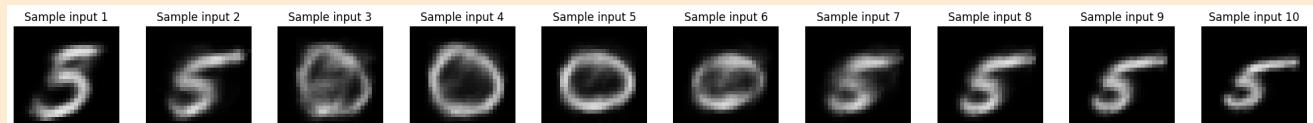
INTERPOLATION

Same Class

Geodesic Interpolation

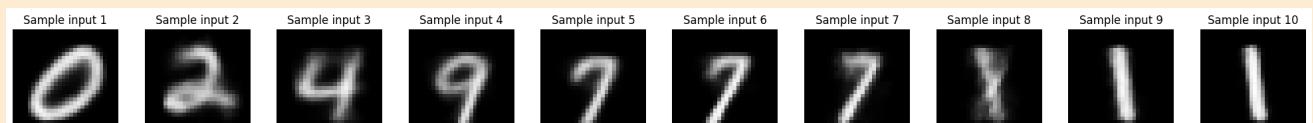


Euclidean Interpolation

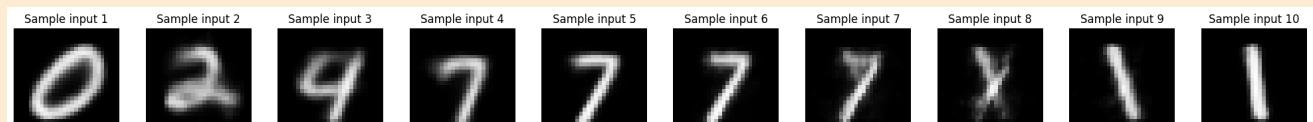


Different Class

Geodesic Interpolation



Euclidean Interpolation

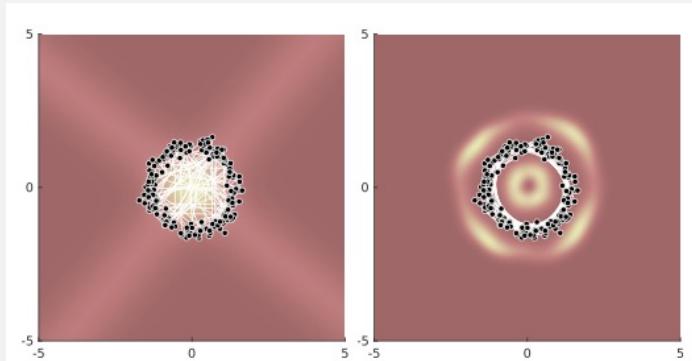


RANDOM MANIFOLDS

Goal of regularization: To smooth the function and ease optimization but with the side effect of creating smooth manifolds, lacking information about holes and such.

Solution: Random manifolds.

$$\bar{\mathbf{M}}_{\mathbf{z}} = \mathbb{E}_{p(\epsilon)}[\mathbf{M}_{\mathbf{z}}] = (\mathbf{J}_{\mathbf{z}}^{(\mu)})^T (\mathbf{J}_{\mathbf{z}}^{(\mu)}) + (\mathbf{J}_{\mathbf{z}}^{(\sigma)})^T (\mathbf{J}_{\mathbf{z}}^{(\sigma)})$$



Deterministic Embedded Manifold Stochastic/Random Embedded Manifold

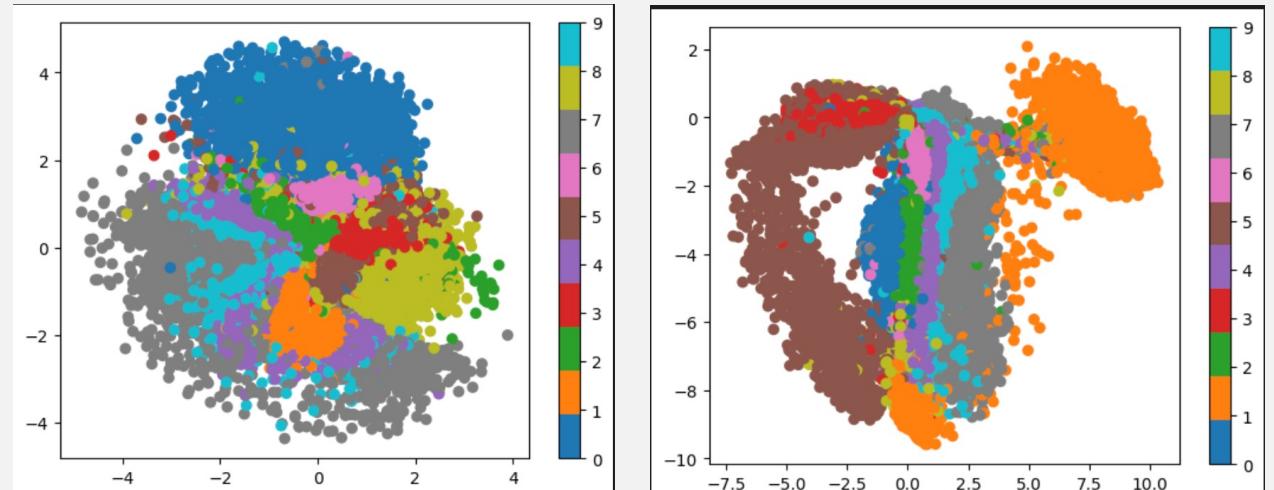
ISOMETRIC REPRESENTATION VAE (IRVAE)

Goal: Preserve Euclidean Relationship

How: Isotropic Learnable Gaussian + Scaled
Isometric Regularization Term in Loss Function

Paper:

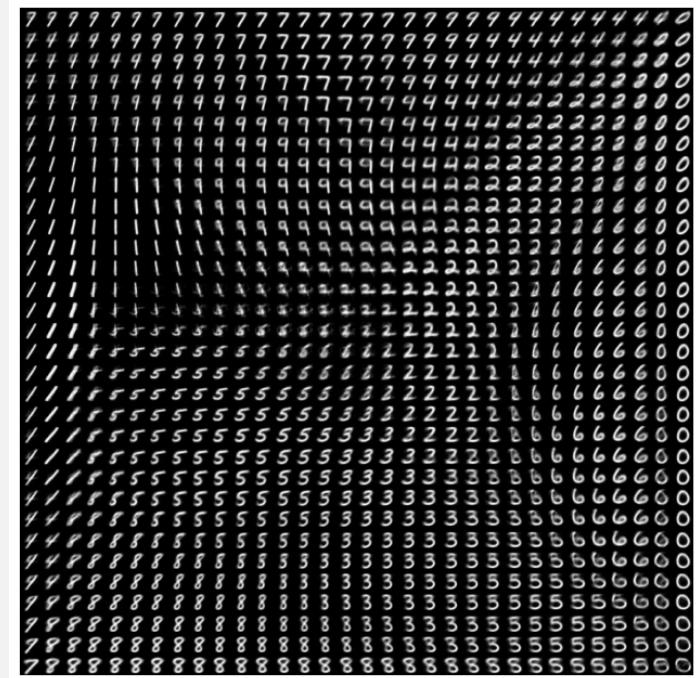
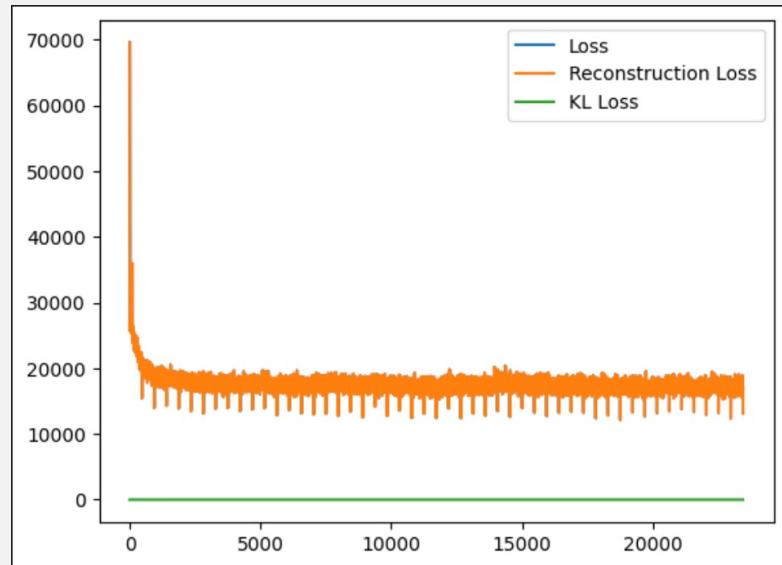
Regularized Autoencoders for Isometric
Representation Learning – Lee et. al 2022



Simple VAE

IRVAE

TRAINING IRVAE



RADIAL BASIS FUNCTION NETWORK (RBFNET)

What: Network that combines radial kernels to approximate a target function.

How

Initialize the centers of radial kernels using k-means. Then, bandwidths ("decay rate") for the radial kernels are generated. Finally, inference involves calculating the distance between a data point and the centers and weighting it using the bandwidths.

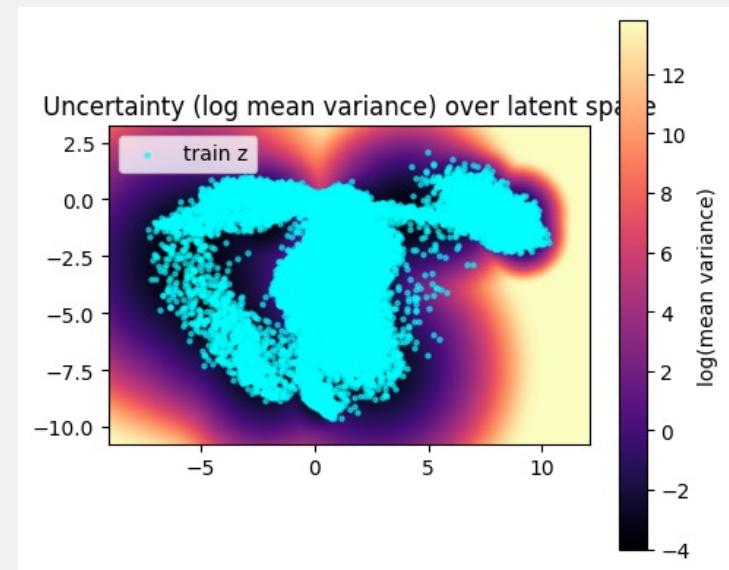
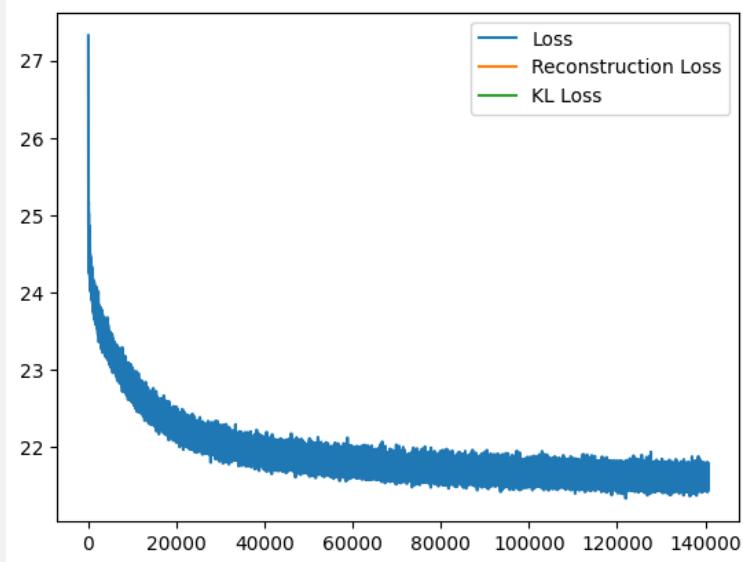
Why

- Controllable decay rate and tolerance towards out-of-distribution data.
- Often used to model VAE uncertainty

Paper Inspiration:

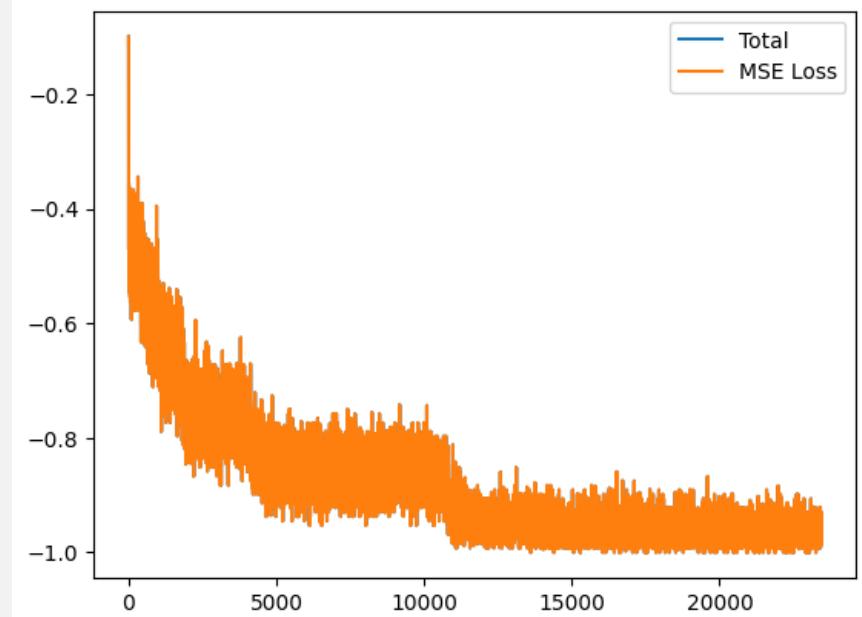
Back to the Future: Radial Basis Function Network Revisited – Que et. al 2020

TRAINING RBFNET



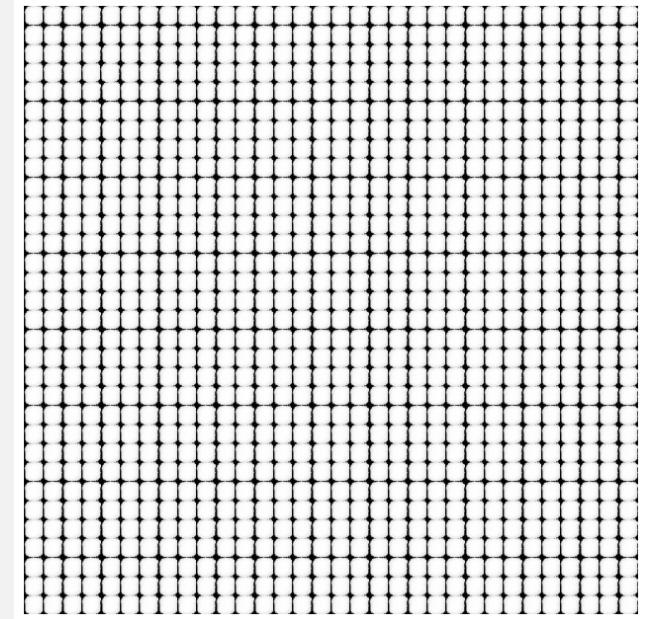
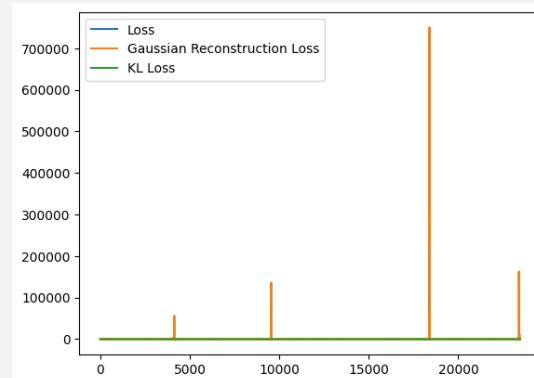
DISCRIMINATIVE CNN MODEL

```
CustomCNN(  
    (layers): Sequential(  
        (0): Conv2d(1, 16, kernel_size=(3, 3), stride=(1, 1))  
        (1): LayerNorm((26,), eps=1e-05, elementwise_affine=True)  
        (2): ReLU(inplace=True)  
        (3): MaxPool2d(kernel_size=2, stride=2, padding=0, dilation=1, ceil_mode=False)  
        (4): Flatten(start_dim=1, end_dim=-1)  
        (5): LazyLinear(in_features=0, out_features=128, bias=True)  
        (6): ReLU(inplace=True)  
        (7): Linear(in_features=128, out_features=10, bias=True)  
        (8): Softmax(dim=1)  
    )  
    (loss_func): NLLLoss()  
)
```



OTHER (FAILED) EXPERIMENTS

- Gaussian Uncertainty VAE
- Hierarchical VAE
- Gaussian Process Variational Latent Model (GPVLM)

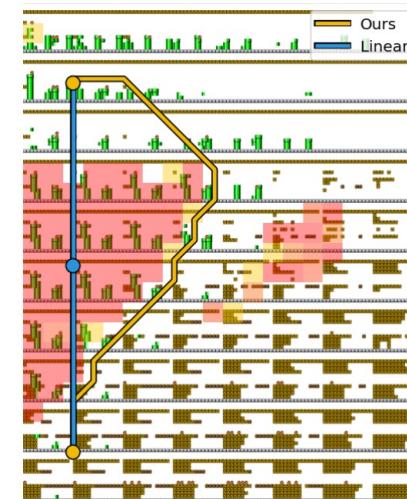


COOL RELATED WORK

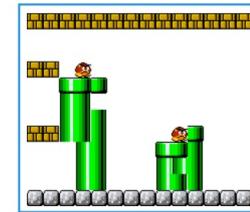
Mario Plays on a Manifold: Generating Functional Content in Latent Space through Differential Geometry - Gonzalez-Duque et. al 2022

Data Generation in Low Sample Size Setting Using Manifold Sampling and a Geometry-Aware VAE - Chadebec et. al 2021

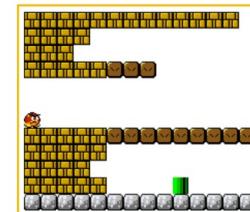
Latent space of Super Mario Bros



Not Functional

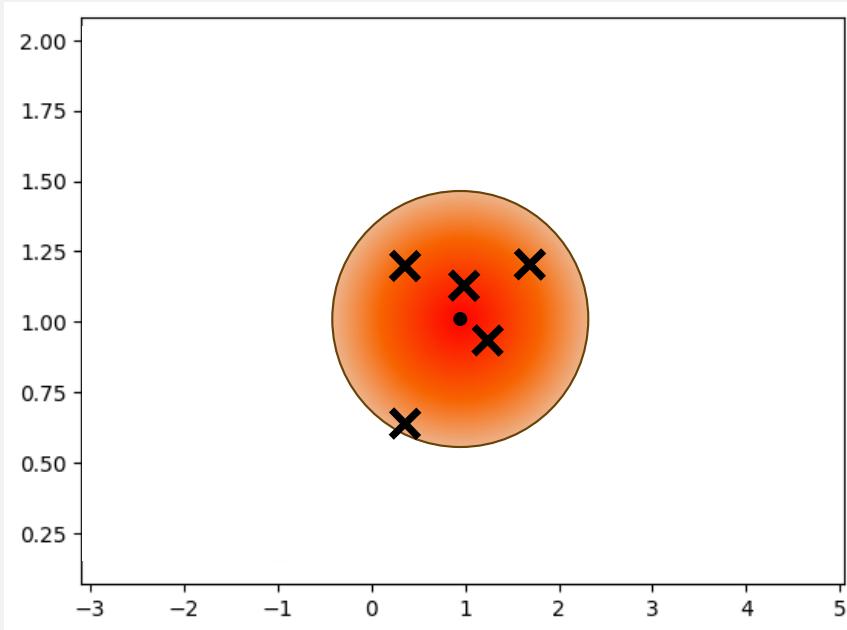


Functional



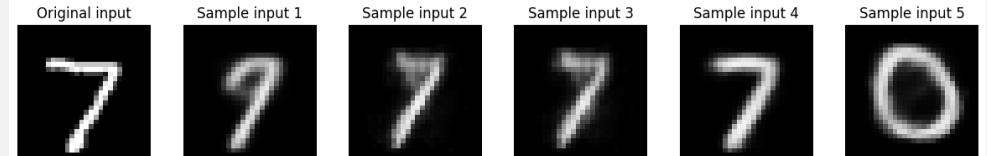
SAMPLING

GAUSSIAN SAMPLING

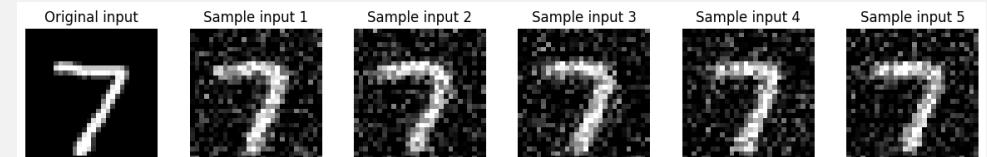


VAE Examples

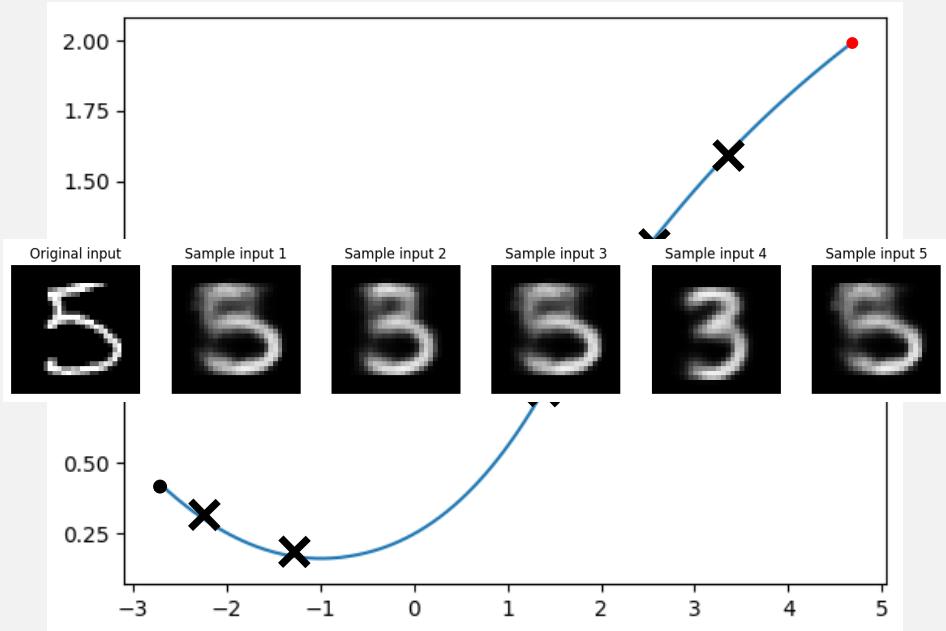
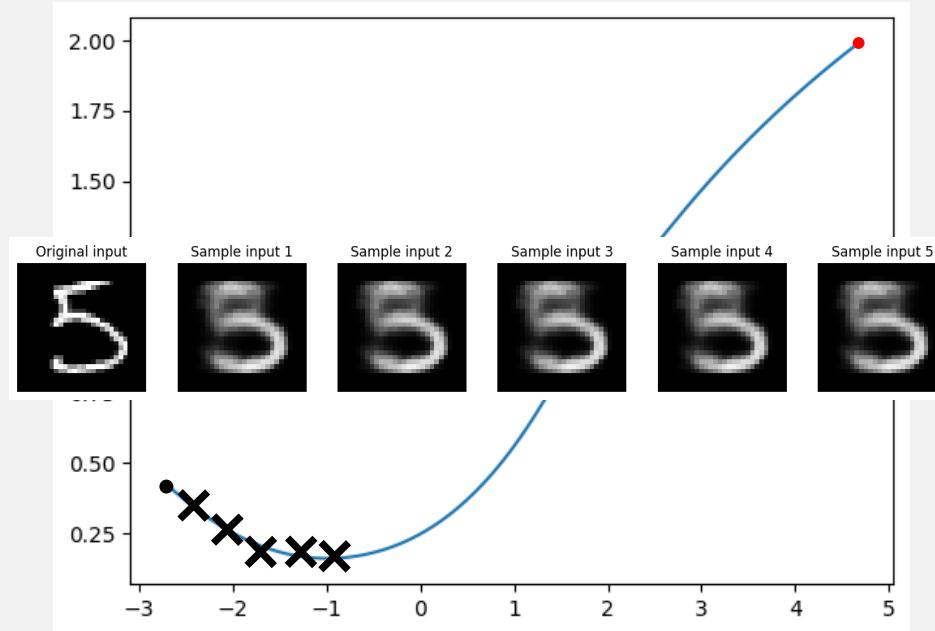
Latent Space



Observation Space



GEODESIC SAMPLING



Red – Latent sample from
predicted class

UNCERTAINTY

METRICS

- Variance
- Coefficient of Variation (Relative STD)
- Entropy
- Percent Entropy

$$CV = \frac{\sigma}{\mu}$$

$$H(X) := - \sum_{x \in \mathcal{X}} p(x) \log p(x)$$

UNCERTAINTY FROM GEODESIC SAMPLING

Mispredictions

```
Prediction on samples: [3, 5, 3, 3, 0]
Variance of prediction: 2.56
Coefficient of variation: 0.5714285693877552
Entropy of prediction: 2.270611524581909
Entropy as percent: 98.6%
```

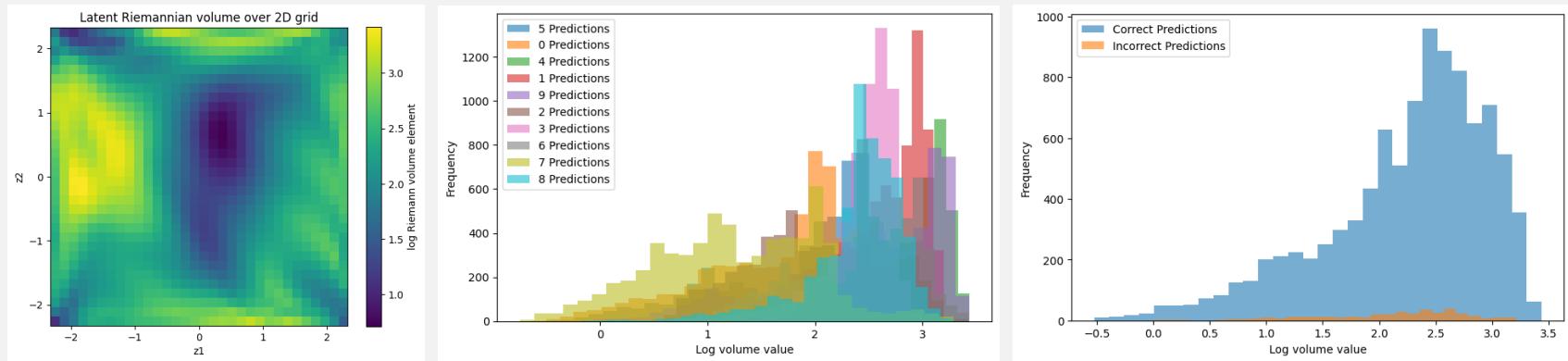
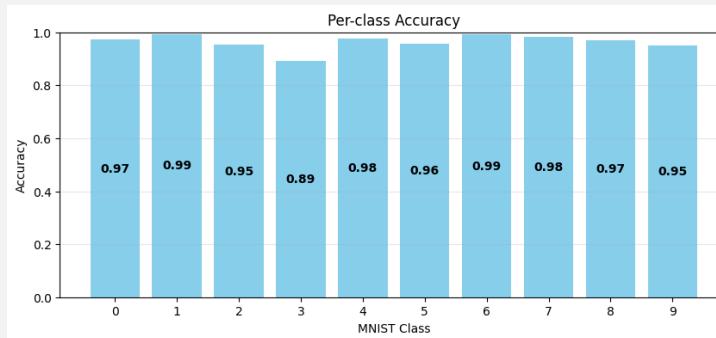
```
----- Average uncertainty values for mispredictions -----
Variance of prediction: 1.0560000000000003
Coefficient of variation: 0.09364875324704096
Entropy of prediction: 2.2392616271972656
Entropy as percent: 97.2%
```

Correct Predictions

```
Prediction on samples: [7, 7, 7, 7, 7]
Variance of prediction: 0.0
Coefficient of variation: 0.0
Entropy of prediction: 2.2291808128356934
Entropy as percent: 96.8%
```

```
----- Average uncertainty values for correct predictions -----
Variance of prediction: 0.09600000000000002
Coefficient of variation: 0.0544331050927756
Entropy of prediction: 2.2332890033721924
Entropy as percent: 97.0%
```

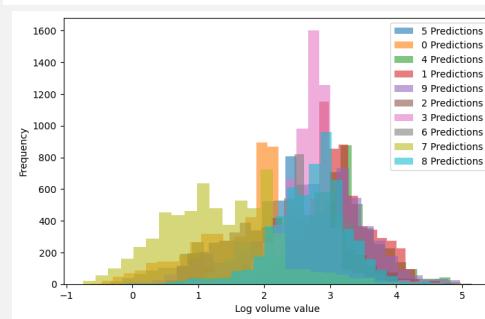
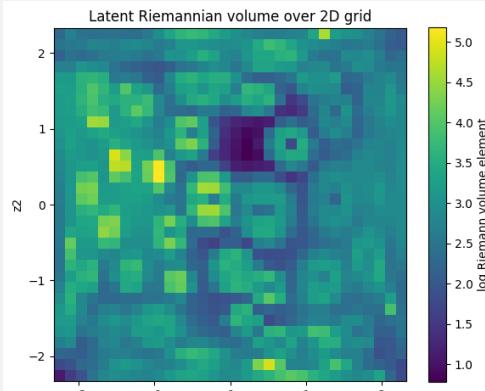
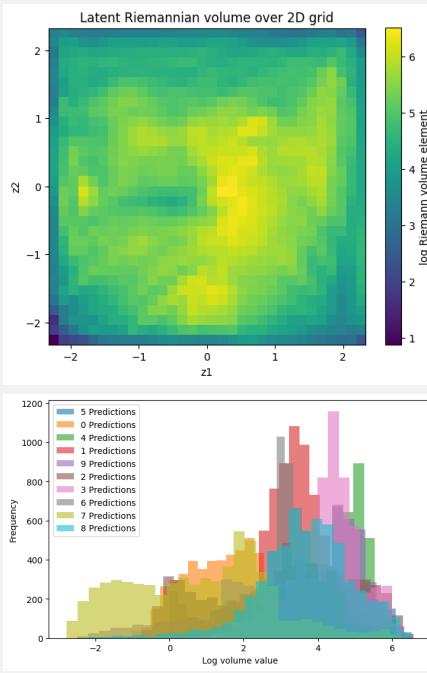
UNCERTAINTY FROM LOG OF VOLUME METRIC



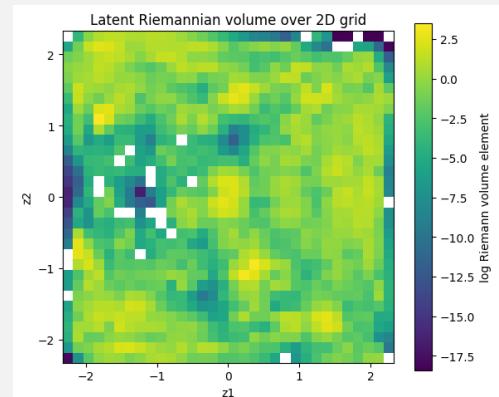
UNCERTAINTY FROM LOG OF VOLUME METRIC

VAE+RBF (Random Manifold)

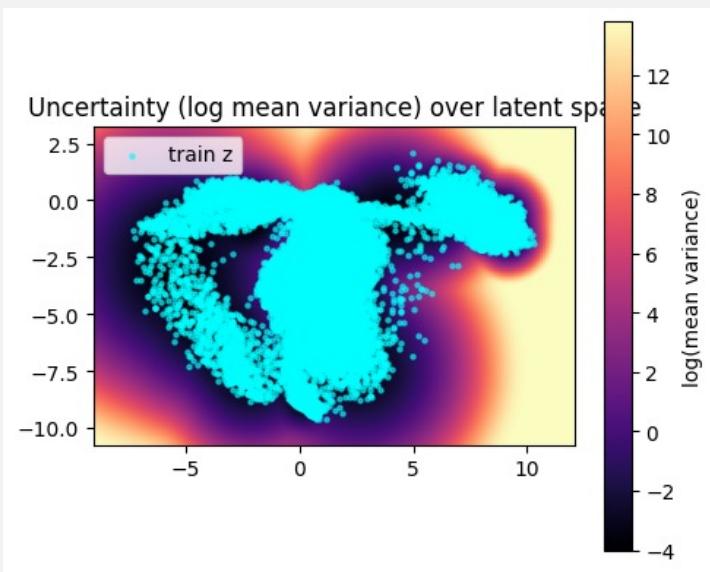
IRVAE



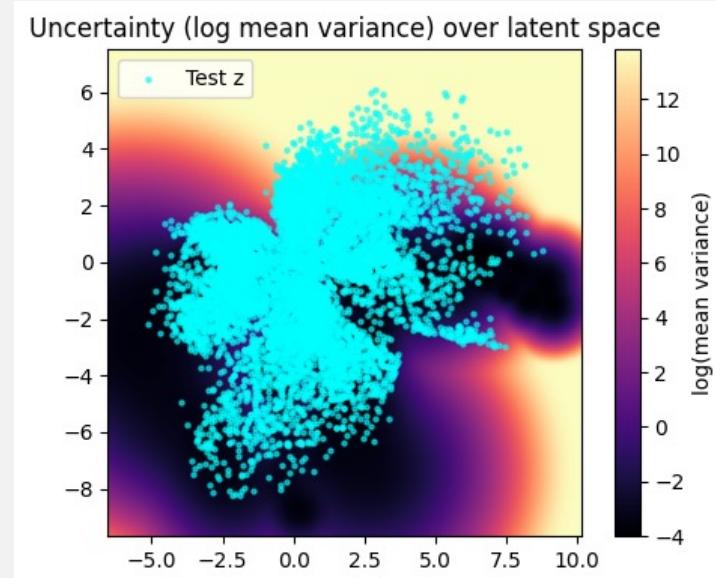
RBFNet



UNCERTAINTY FROM TRAINED RBFNET



Train Dataset



Test Dataset

FUTURE DIRECTIONS

- Experiment with using the average intraclass geodesic length as a metric for uncertainty
- GPLVM Experimentation
- Look at higher dimensionality latent spaces

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- <https://github.com/MachineLearningLifeScience/stochman>