STATISTICAL DATA DEPTH IN DEEP LEARNING: APPLICATION TO OUT OF DISTRIBUTION DETECTION

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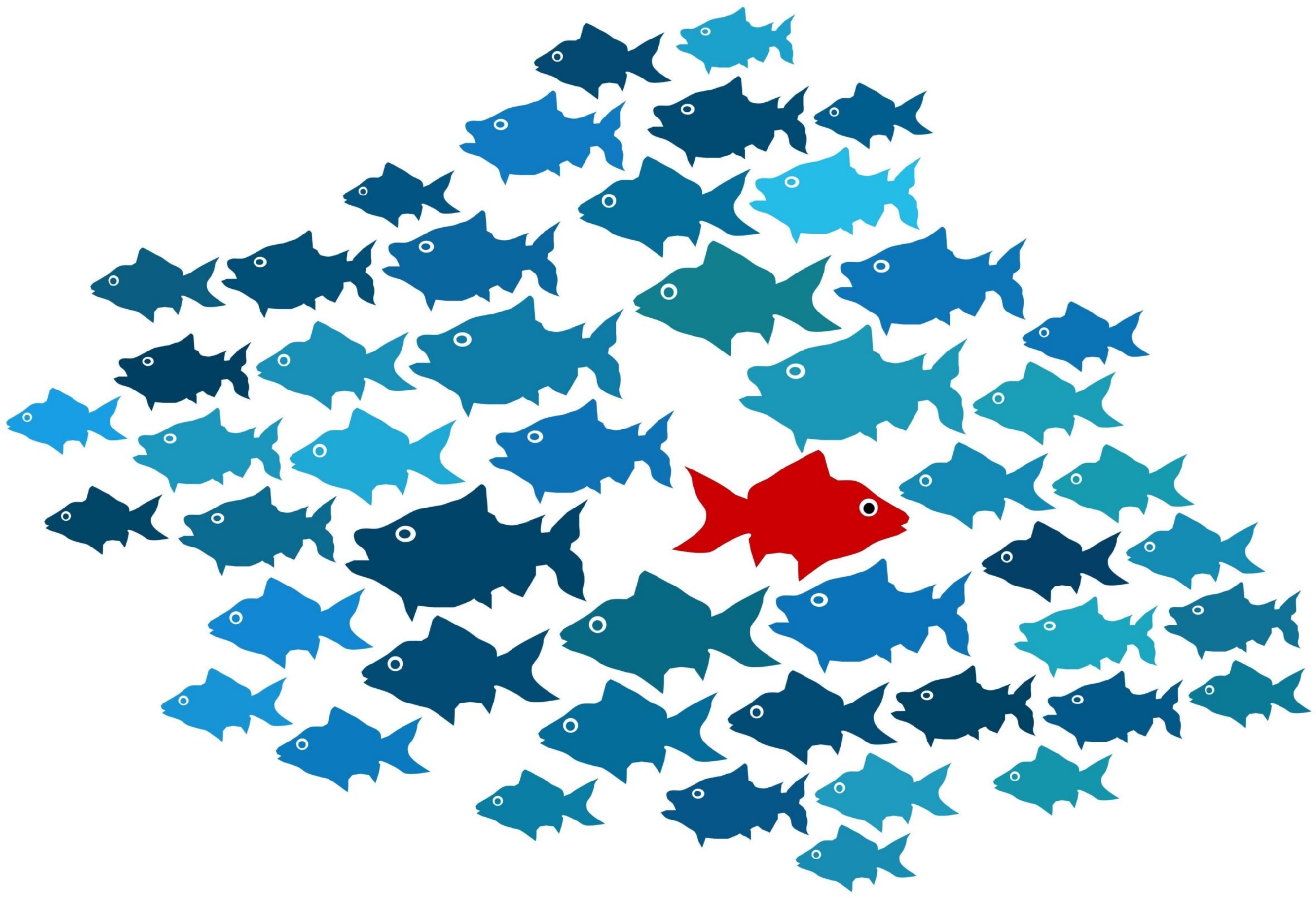
INTRODUCTION

OUT OF DISTRIBUTION DETECTION

A model's ability to recognize and appropriately handle data that deviates significantly from its training set.

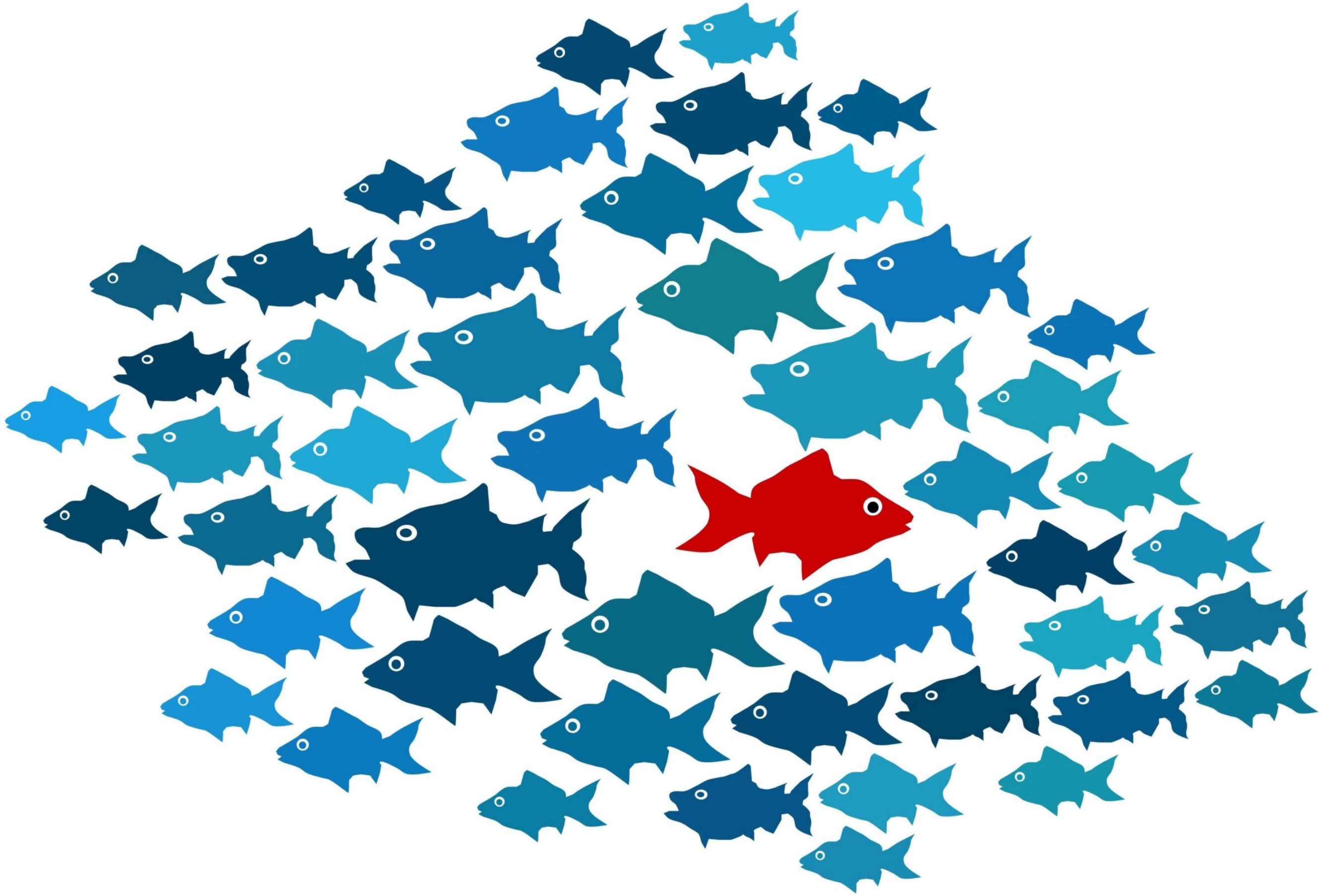
Importance:

- Error Reduction
- Data Quality Control
- Model Robustness
- Safety and Reliability



OUT OF DISTRIBUTION DETECTION – CHALLENGES

- Defining “Out-of-Distribution”
- High Dimensionality
- Computation Costs
- Domain Shift
- Model Calibration
- Noise and Outliers
- Transferability
- Evaluation Metrics



STATISTICAL DATA DEPTH

A **data depth** measures how close a given point is located to the center of a distribution. For $x \in \mathbb{R}^p$ and a p-variate random vector X distributed as $P \in \mathcal{P}$, a data depth is a function

$$D : \mathbb{R}^p \times \mathcal{P} \to [0,1], \qquad (\boldsymbol{x}, P) \longmapsto D(\boldsymbol{x}|P)$$

that is :

D1 **translation invariant:** $D(\boldsymbol{x} + b \,|X + b) = D(\boldsymbol{x}|X)$ for any $b \in \mathbb{R}^p$;

D2 **linear invariant:** $D(A\boldsymbol{x} \,|AX) = D(\boldsymbol{x}|X)$ for any $p \times p$ non-singular matrix A;

D3 **vanishing at infinity:** $\lim_{\|\boldsymbol{x}\| \to \infty} D(\boldsymbol{x}|X) = 0$;

D4 **monotone on rays:** for any $\boldsymbol{x}^* \in \arg\max_{\boldsymbol{x} \in \mathbb{R}^p} D(\boldsymbol{x}|X)$, any $x \in \mathbb{R}^p$, and any $0 \leq \alpha \leq 1$ it holds: $D(\boldsymbol{x}|X) \leq D(\boldsymbol{x}^* + \alpha(\boldsymbol{x} - \boldsymbol{x}^*)|X)$;

D5 **upper semicontinuous in $\boldsymbol{x}$:** the upper-level sets $D_\alpha(\boldsymbol{x}|X) \leq \{\boldsymbol{x} \in \mathbb{R}^p : D(\boldsymbol{x}|X) \geq \alpha\}$ are closed for all α.

STATISTICAL DATA DEPTH

There are many definitions of data depth:

- Mahalanobis depth (Mahalanobis, 1936)
- Convex hull peeling depth (Barnett, 1976; Eddy, 1981)
- Projection depth (Stahel, 1981; Donoho, 1982)
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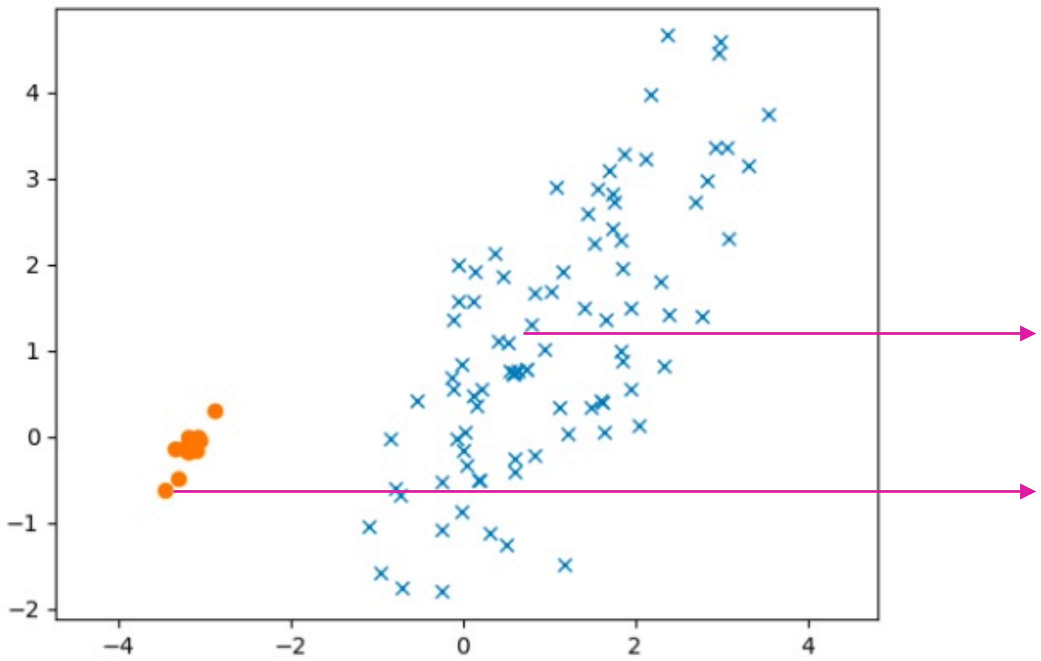
STATISTICAL DATA DEPTH – BIVARIATE DEMO



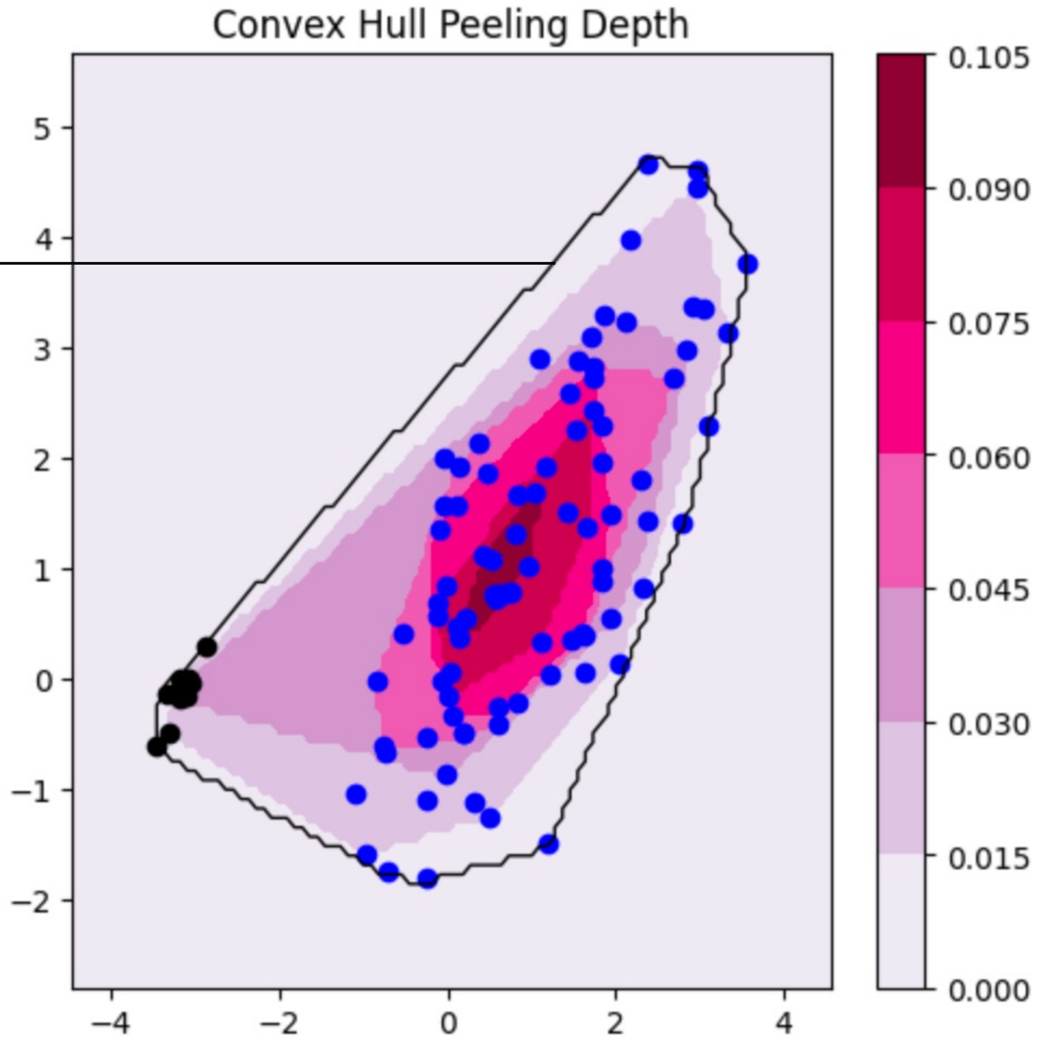
$$\sim \text{Norm}\left(\begin{pmatrix}1\\1\end{pmatrix}, \begin{pmatrix}1 & 1\\1 & 2\end{pmatrix}\right)$$

$$\sim \text{Norm}\left(\begin{pmatrix}-3.181\\-0.222\end{pmatrix}, \frac{1}{36}\begin{pmatrix}1 & 1\\1 & 2\end{pmatrix}\right)$$

Synthetic data generated using two different multivariate normal distributions.

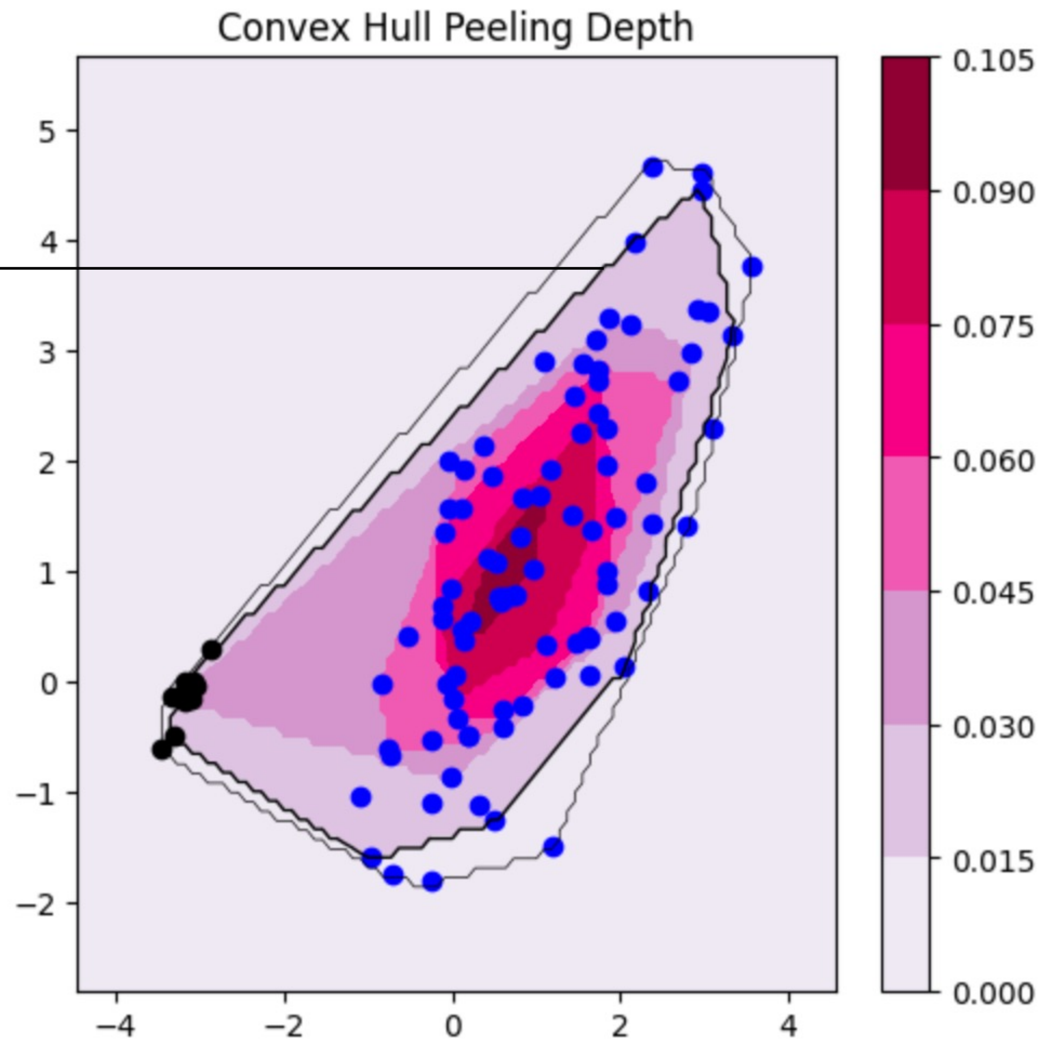
STATISTICAL DATA DEPTH – BIVARIATE DEMO

Outermost convex hull;
Corresponds to data depth ~ 0



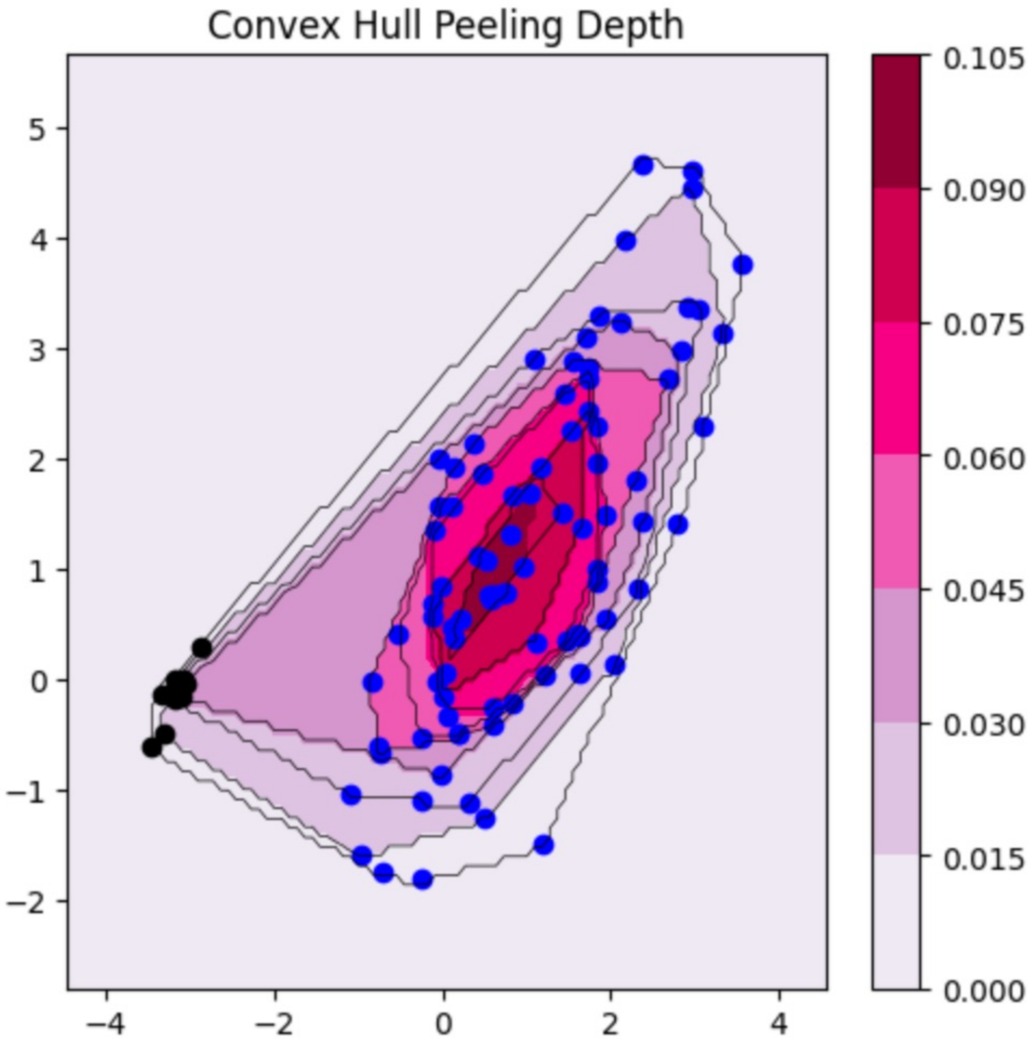
STATISTICAL DATA DEPTH – BIVARIATE DEMO

Next convex hull;
Data depth is now ~ 0.15



STATISTICAL DATA DEPTH - BIVARIATE DEMO

At each level, we construct a new convex hull and assign data depth values accordingly.



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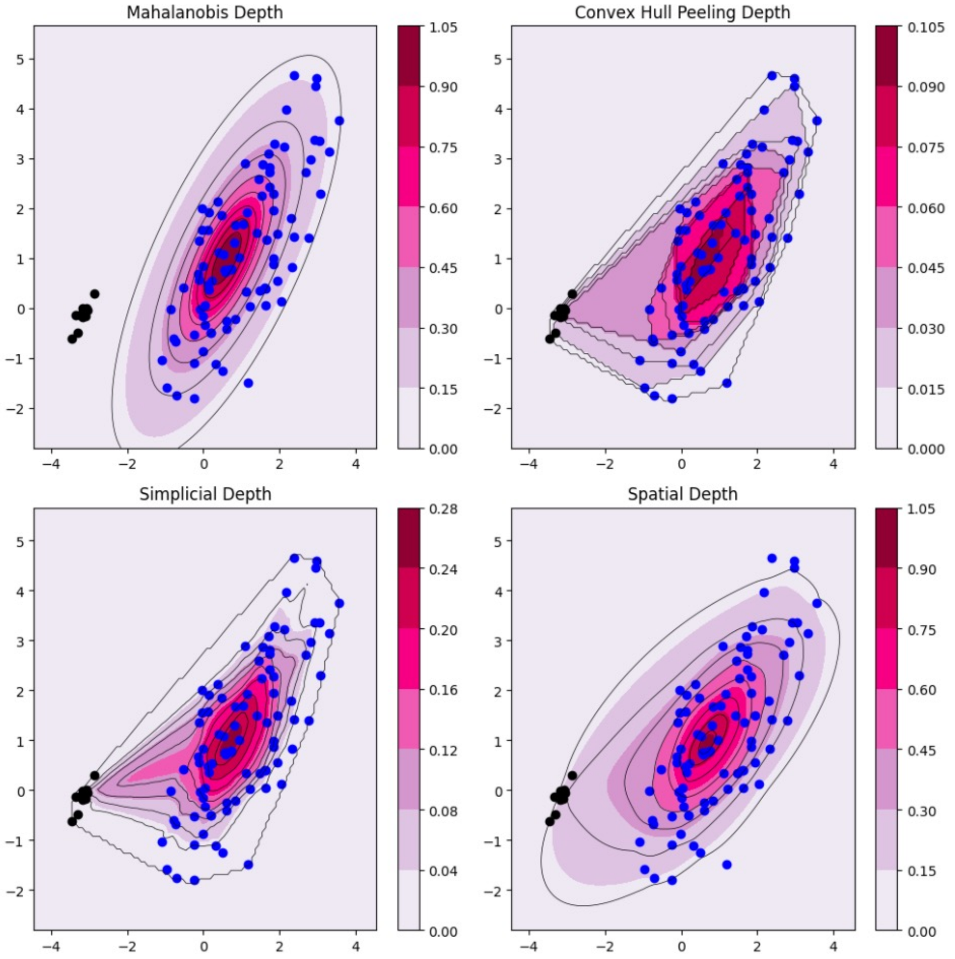
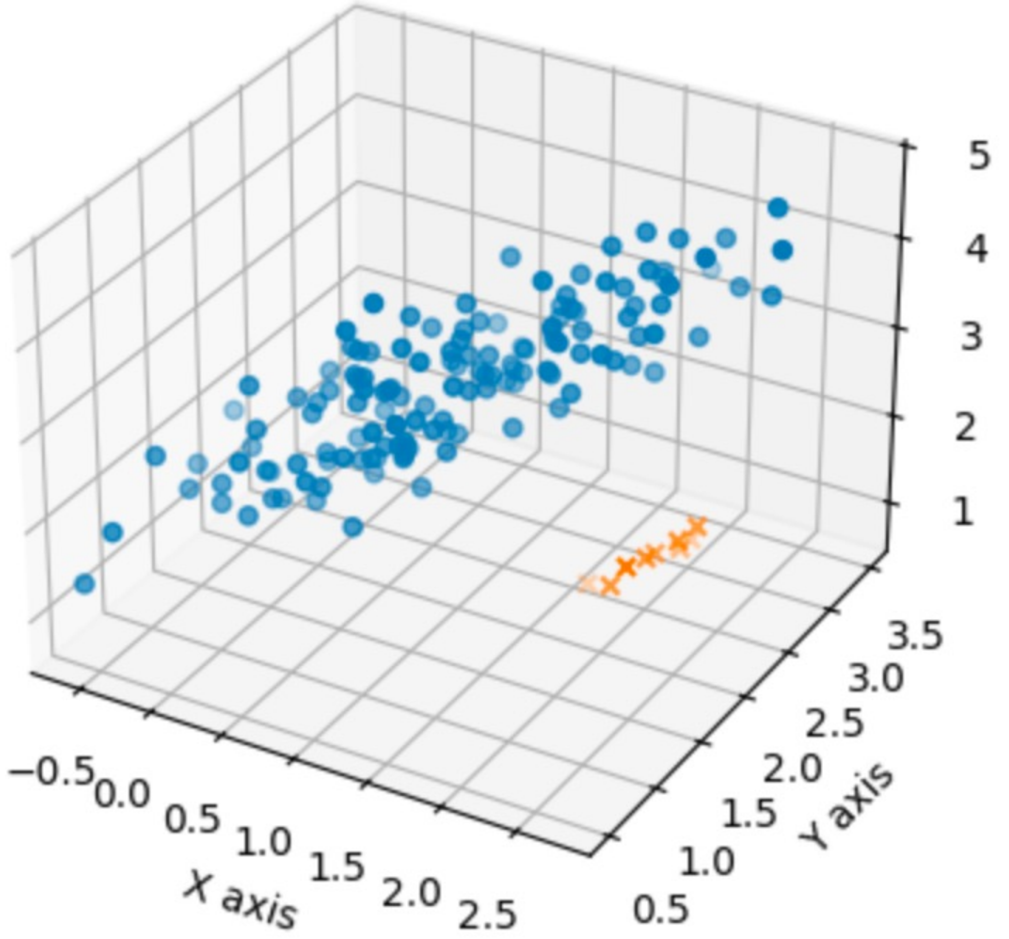


STATISTICAL DATA DEPTH – MULTIVARIATE DEMO



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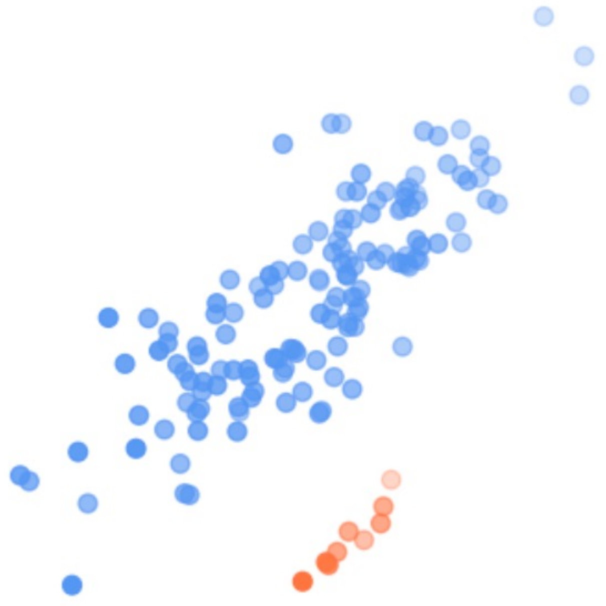

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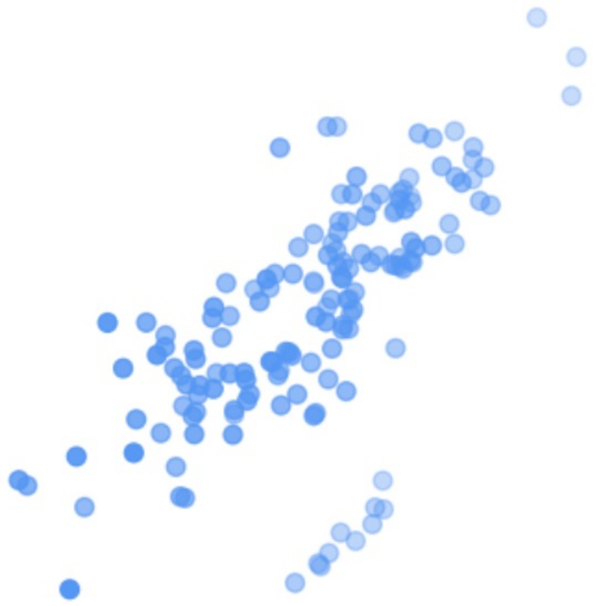

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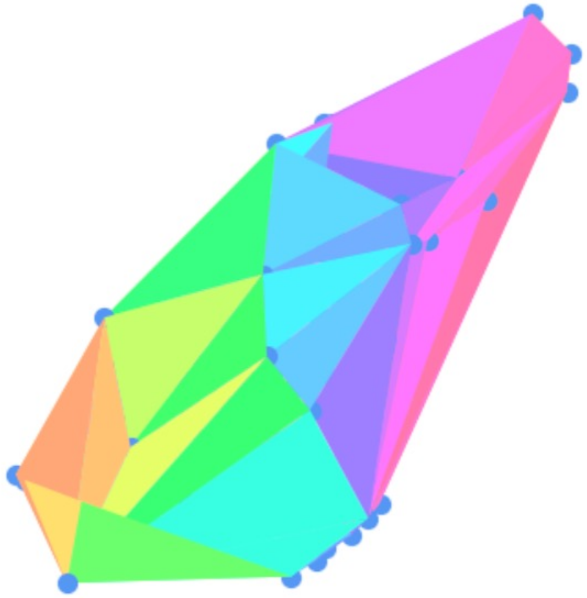

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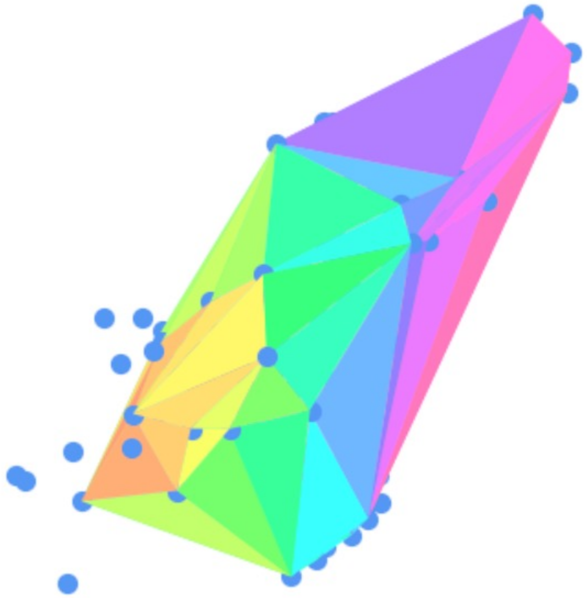

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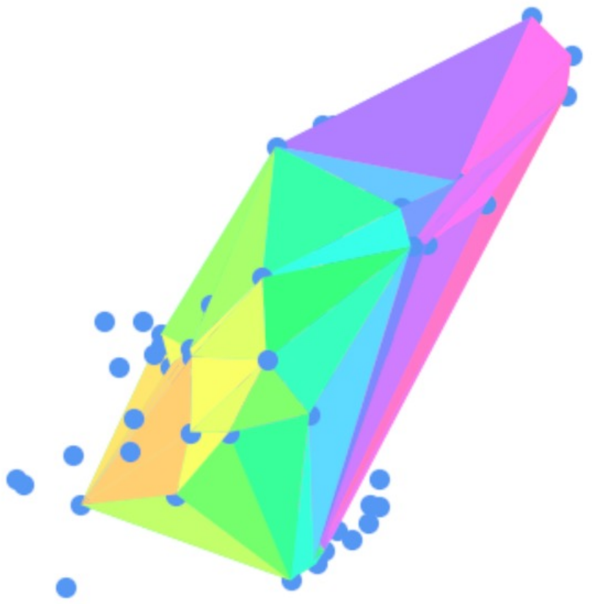

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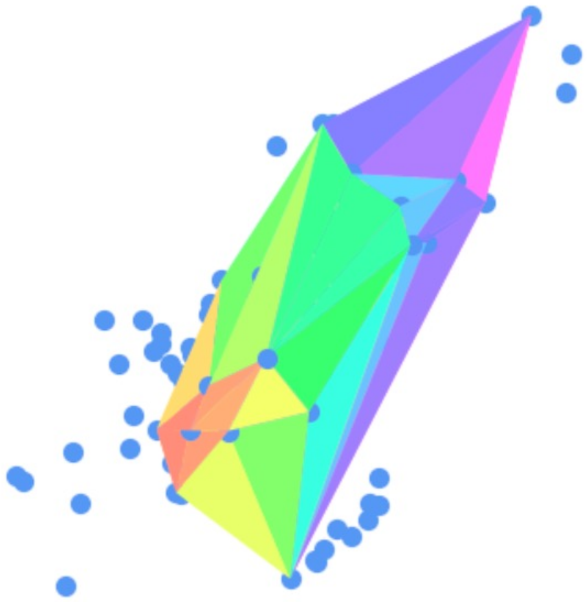

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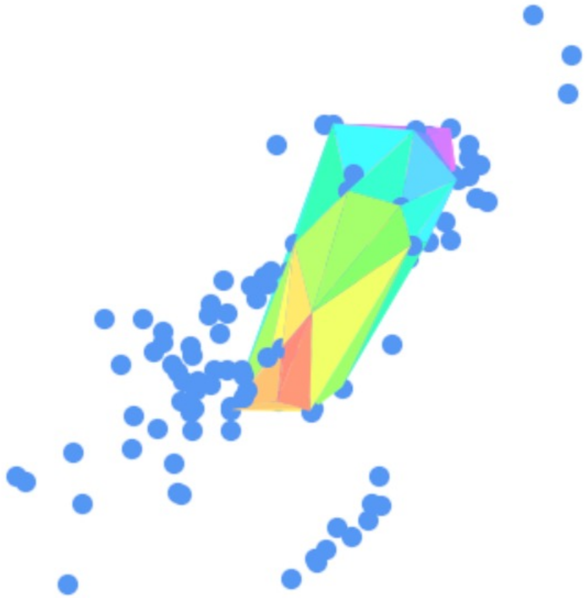

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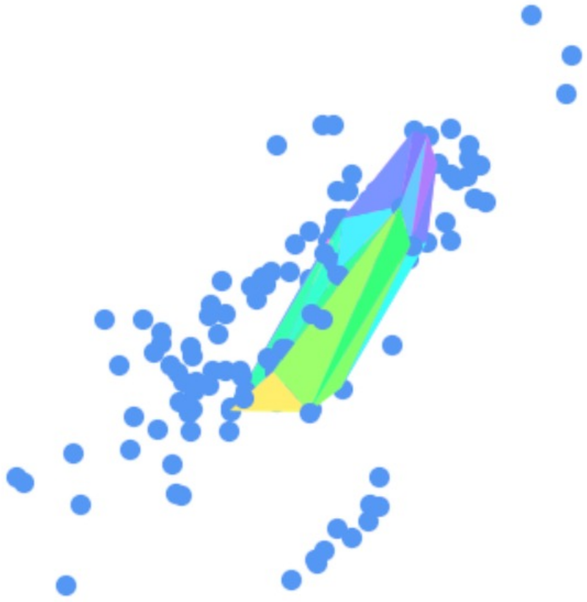

STATISTICAL DATA DEPTH - CHALLENGES

- High Dimensionality
- Scalability
- Robustness
- Choice of Depth Measure
- Non-Euclidean Data
- Interpretability
- Computation of Depth Regions
- Integration with Machine Learning Models

CURRENT CHALLENGES

Out of Distribution Detection

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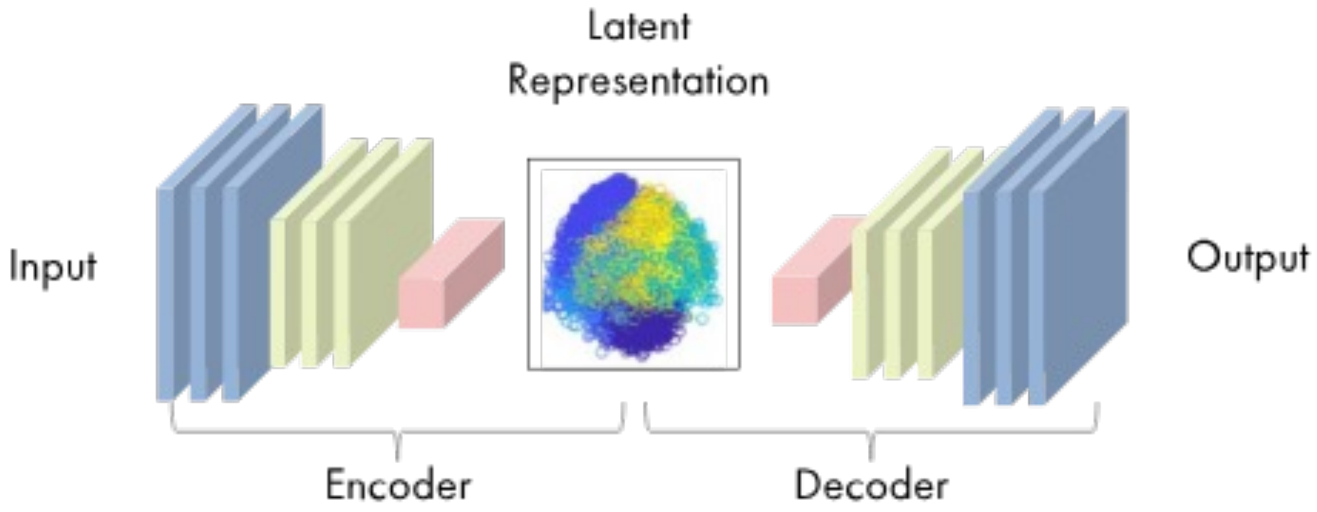
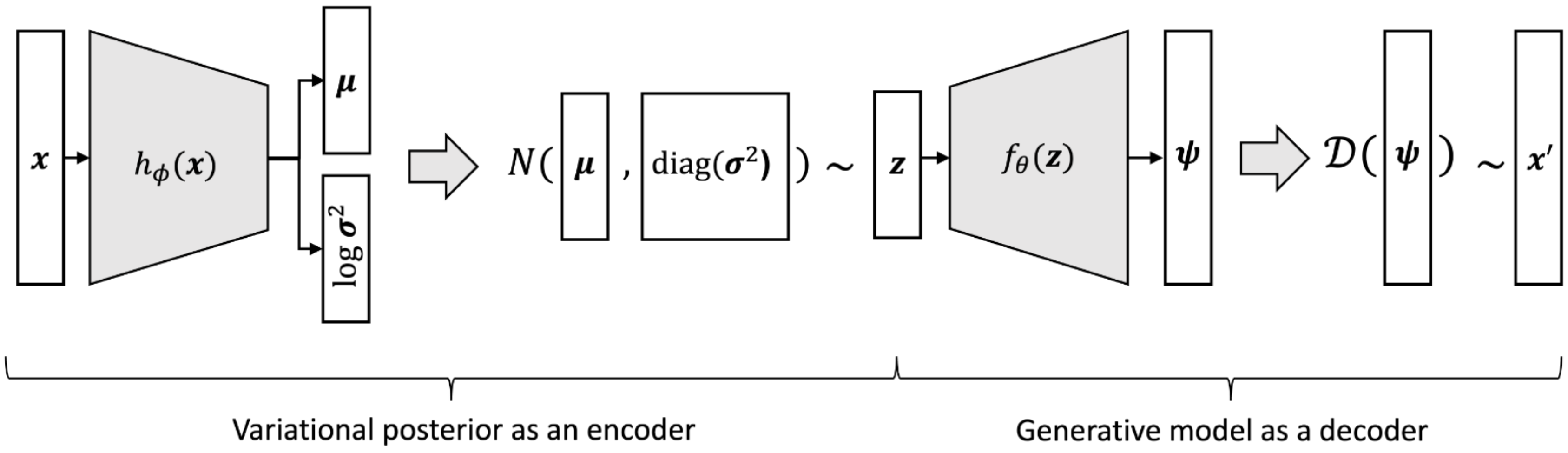
AUTOENCODERS

- A representation learning algorithm
- Learn to map examples to low-dimensional representation



VARIATIONAL AUTOENCODERS

- Variational autoencoders (VAEs), introduced by Kingma and Welling (2013), are a class of probabilistic models that find latent, low-dimensional representations of data.
- VAEs are thus a method for performing dimensionality reduction to reduce data down to their intrinsic dimensionality.



VARIATIONAL AUTOENCODERS – DEMO

- Encoder with two linear layers that produce the mean and log-variance of the latent variables
- Reparameterization trick to ensure differentiability when sampling latent variables.

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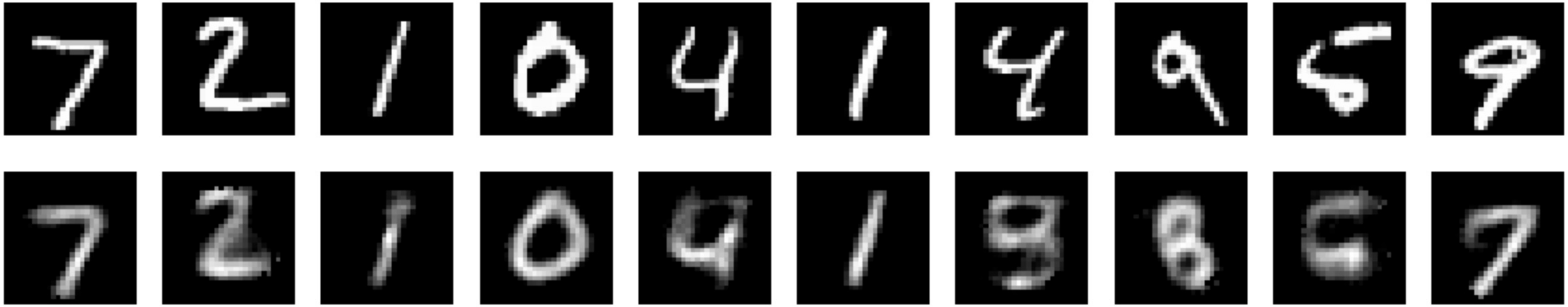

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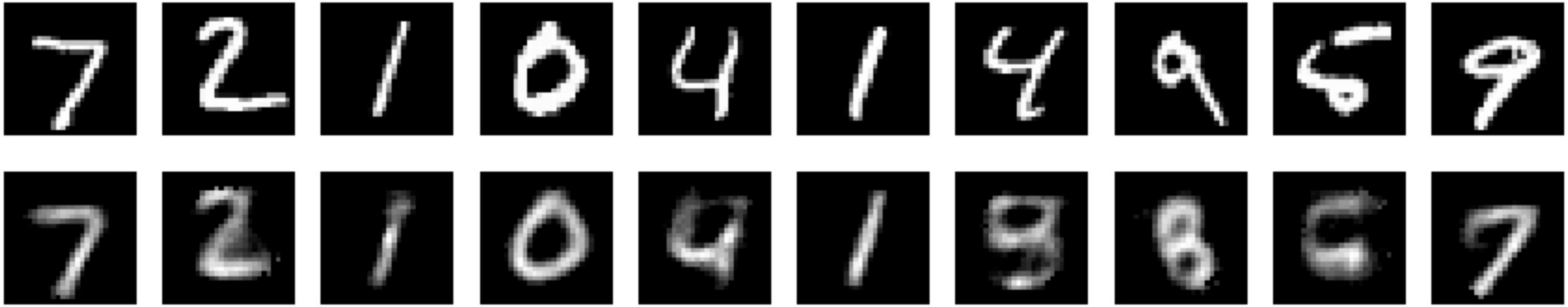
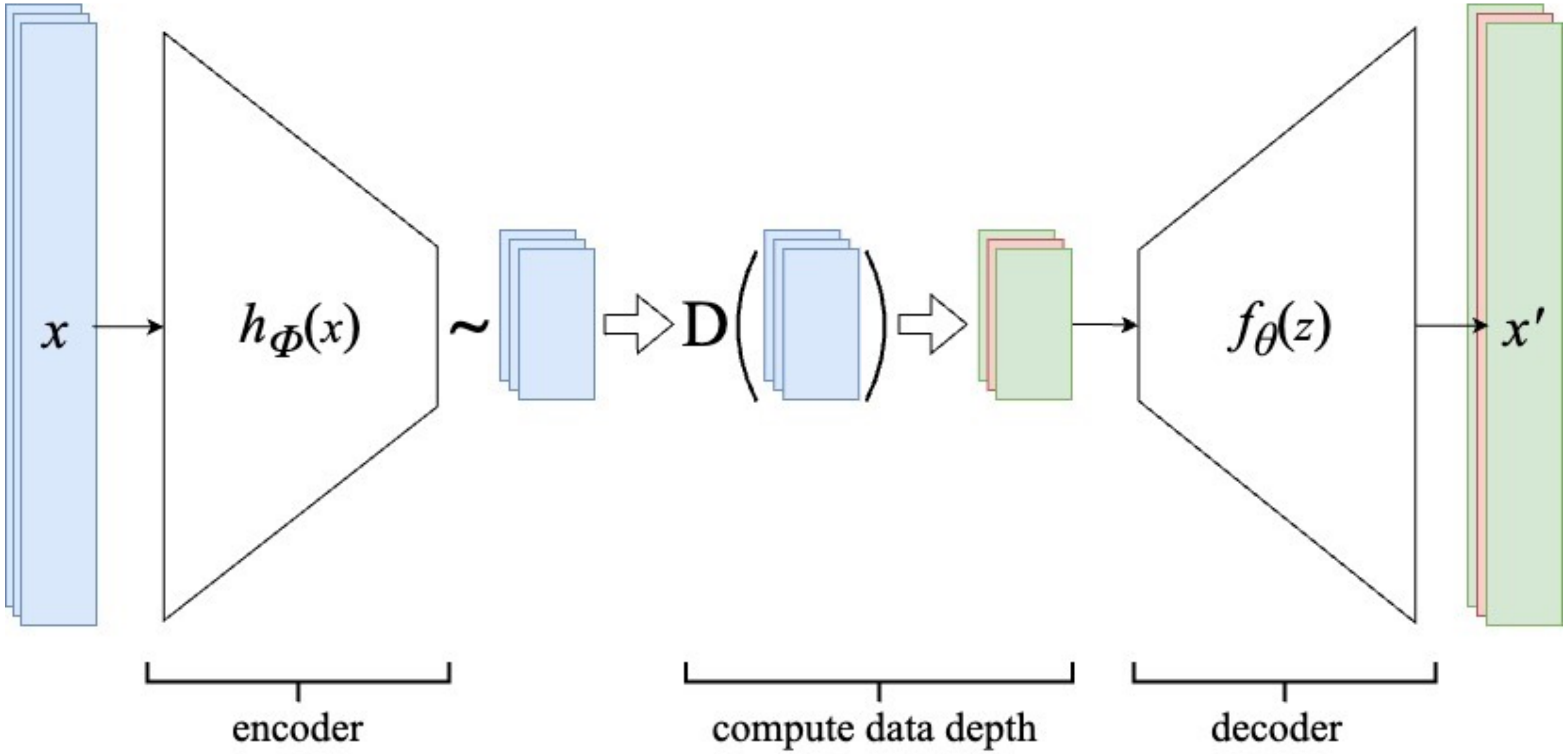


- A combination of reconstruction loss (MSE) and KL divergence to regularize the latent space
- VAE's effectiveness in data compression and latent space representation

VARIATIONAL AUTOENCODERS – KEY ADVANTAGES

- Data generation
- Control of Latent Space
- Modelling Complex Distributions

SOLUTION OVERVIEW



METHODOLOGY

DATASET REVIEW

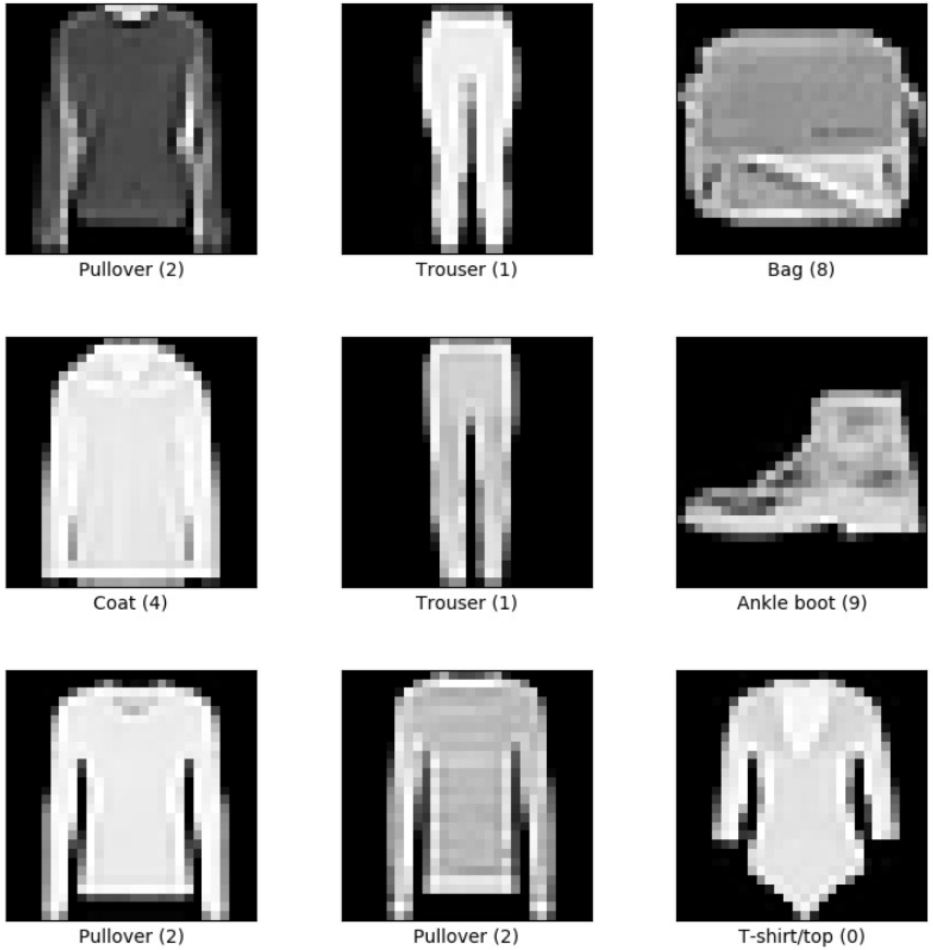
Fashion MNIST Dataset with

Split	Examples
test	10,000
train	60,000

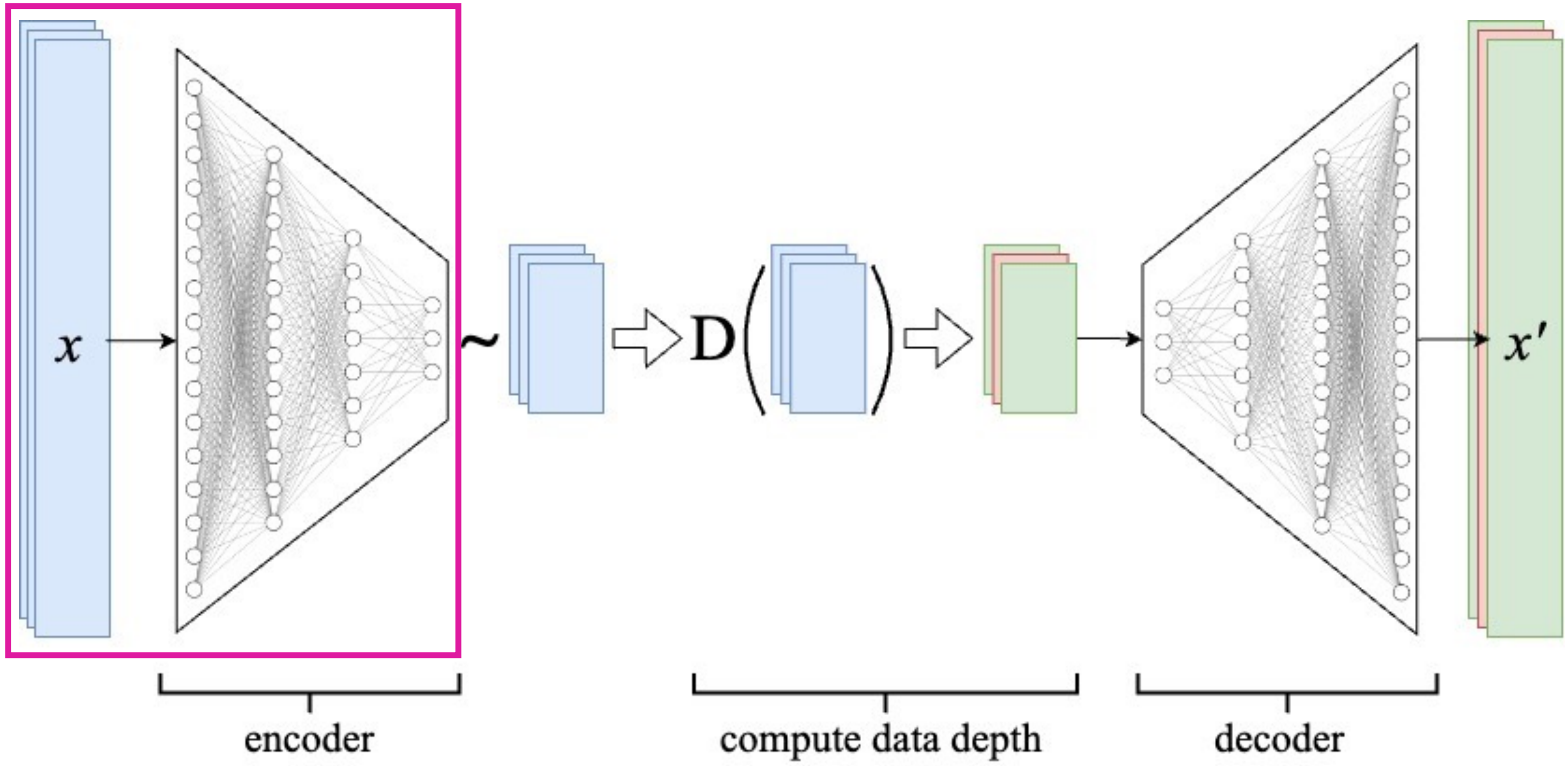
where each example has

```
FeaturesDict({
    'image': Image(shape=(28, 28, 1), dtype=uint8),
    'label': ClassLabel(shape=(), dtype=int64, num_classes=10),
})
```

and each label value corresponds to:



SOLUTION OVERVIEW



We begin by training an encoder on the training dataset of 60000 points to reduce dimensionality.

VARIATIONAL AUTOENCODERS – DEMO

```
class VAE(nn.Module):
    def __init__(self, x_dim, hidden_dim1, hidden_dim2, z_dim=10):
        super(VAE, self).__init__()

        self.encoder = nn.Sequential(
            nn.Linear(x_dim, hidden_dim1),
            nn.ReLU(),
            nn.Linear(hidden_dim1, hidden_dim2),
            nn.ReLU(),
            nn.Linear(hidden_dim2, z_dim * 2)
        )

        self.decoder = nn.Sequential(
            nn.Linear(z_dim, hidden_dim2),
            nn.ReLU(),
            nn.Linear(hidden_dim2, hidden_dim1),
            nn.ReLU(),
            nn.Linear(hidden_dim1, x_dim),
            nn.Sigmoid()
        )
```

VARIATIONAL AUTOENCODERS – DEMO

- Reparametrize function to sample from the latent space by introducing stochasticity.

```
class VAE(nn.Module):
    ...
    def reparameterize(self, mu, logvar):
        std = torch.exp(0.5 * logvar)
        eps = torch.randn_like(std)
        return mu + eps * std

    def forward(self, x):
        h = self.encoder(x)
        mu, logvar = torch.chunk(h, 2, dim=1)
        z = self.reparameterize(mu, logvar)
        return self.decoder(z), z, mu, logvar

# Loss function
def loss_function(reconx, x, mu, logvar):
    BCE = nn.functional.binary_cross_entropy(reconx, x, reduction='sum')
    KLD = -0.5 * torch.sum(1 + logvar - mu.pow(2) - logvar.exp())
    return BCE + KLD
```

VARIATIONAL AUTOENCODERS – DEMO

- Reparametrize function to sample from the latent space by introducing stochasticity.
- The loss function uses a combination of the standard reconstruction loss and KL Divergence loss.

$$\text{loss}_{\text{VAE}}(\varphi, \theta) = -\sum_{i=1}^{n} \mathrm{E}_{z_i \sim q_\varphi(z_i \mid x_i)} \left[\log p_\theta(x_i \mid z_i)\right] - \mathrm{KL}(q_\varphi(z_i \mid x_i) \,||\, p(z_i))$$

```python
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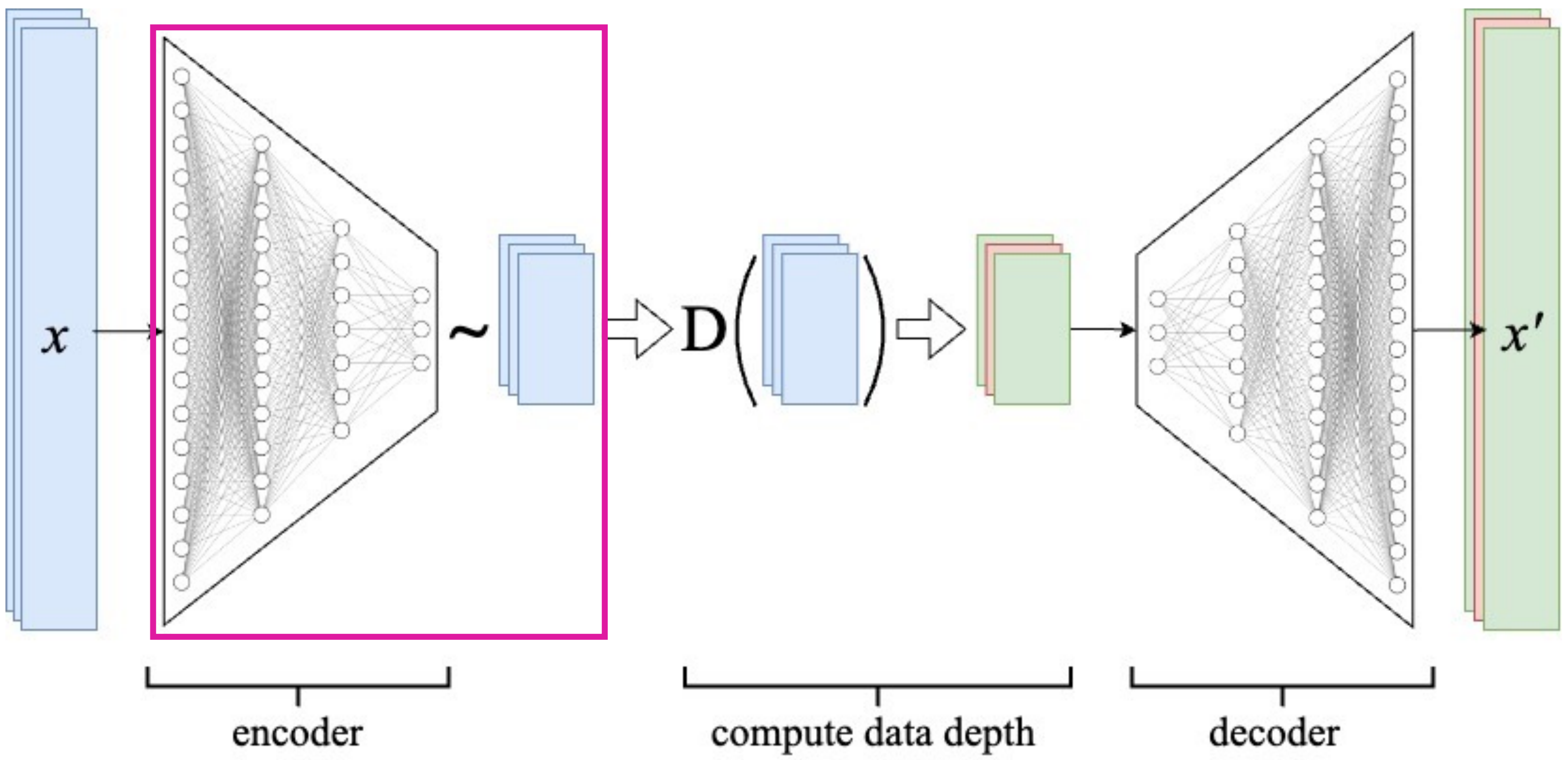


Using the trained encoder, we obtain the latent space representation for each point in the test set.

VARIATIONAL AUTOENCODERS – DEMO

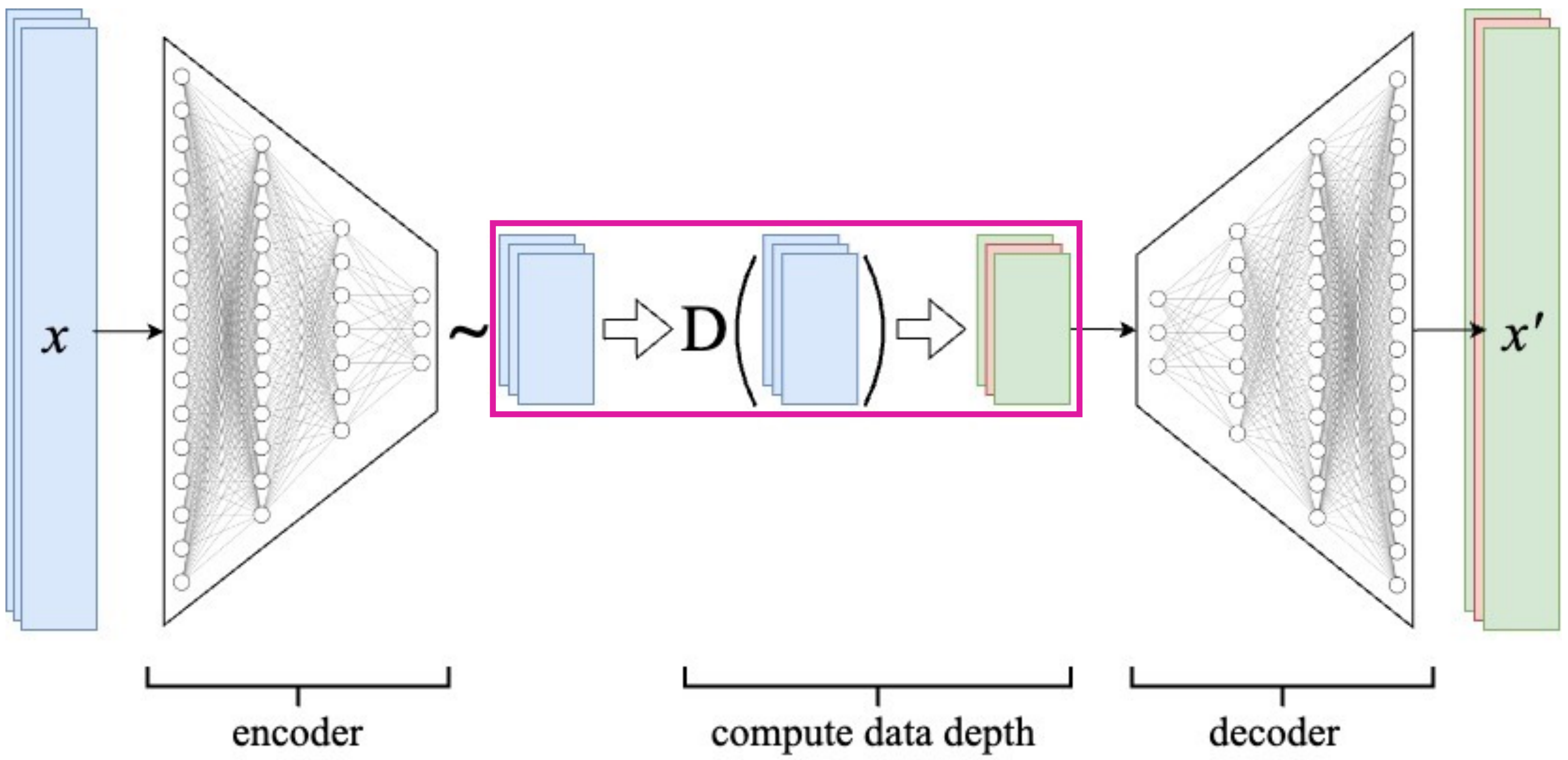
- Evaluate the trained model on the test dataset to obtain the latent representations and store them in a numpy array.

```
trained_model.eval()

# initialize lists to store latent space and their true labels
latent_space = []
labels = []
sample_no = 1 # in case MAX_STEPS is defined
with torch.no_grad():
    for batch in fashion_mnist_test:
        if MAX_STEPS != None and sample_no > MAX_STEPS :
            break
        x, y = batch
        x = x.view(-1, x.size(0))
        _, z, _, _ = trained_model(x)
        latent_space.append(z.cpu().numpy())
        labels.append(torch.tensor(y).cpu().numpy())
        sample_no += 1

latent_space = np.concatenate(latent_space, axis=0)
labels = np.concatenate([labels], axis=0)
```

SOLUTION OVERVIEW



Finally, use the depth function to compute data depth for each point.

VARIATIONAL AUTOENCODERS – DEMO

- Multivariate library to compute data depth using spatial depth (polynomial time).
- Set a threshold to classify points as normal or anomalous.

```
# use multivariate library to compute data depth
depths = spatial(latent_space, latent_space)

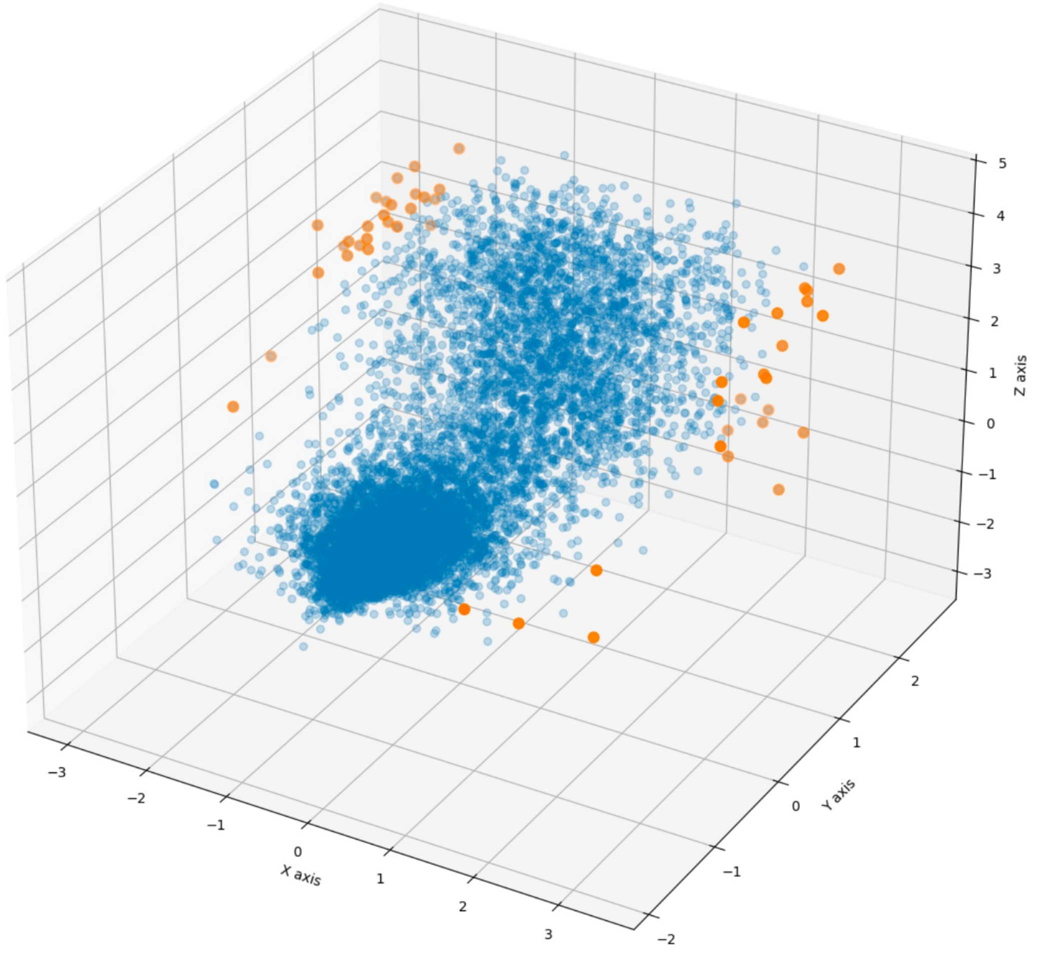
# set a threshold for anomalies (e.g., top 0.5% furthest points)
threshold = np.percentile(depths, 0.5)

# get anomalies
anomalies = depths ⩽ threshold
```

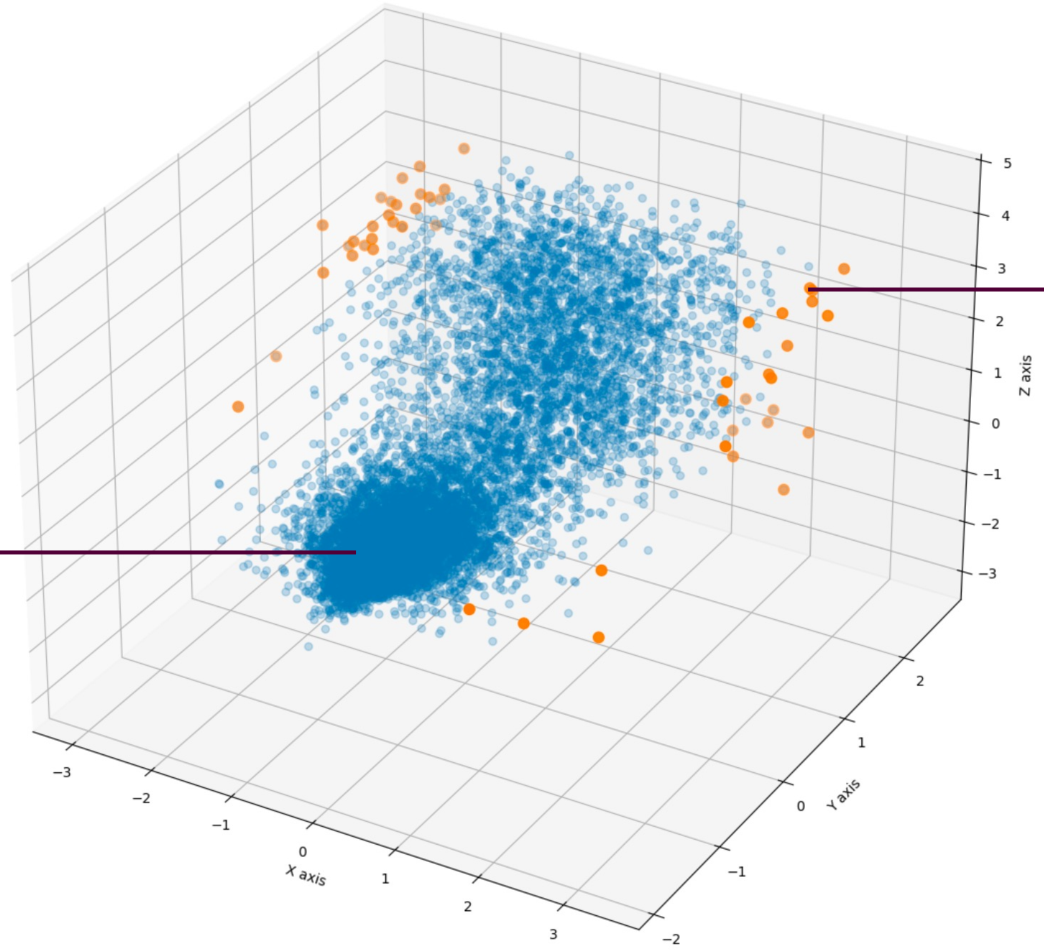
```
Number of points : 10000
Min Data Depth   : 0.03976266539252871
Max Data Depth   : 0.9528853364958756
Std Deviation    : 0.17370466079234456
Threshold        : 0.07019434229670497
```

RESULTS AND ANALYSIS

ANOMALY DISTRIBUTION



ANOMALY DISTRIBUTION



Most anomalies seem to away from the median of the data

The median would be somewhere around here

CONVEX HULL PROGRESSION

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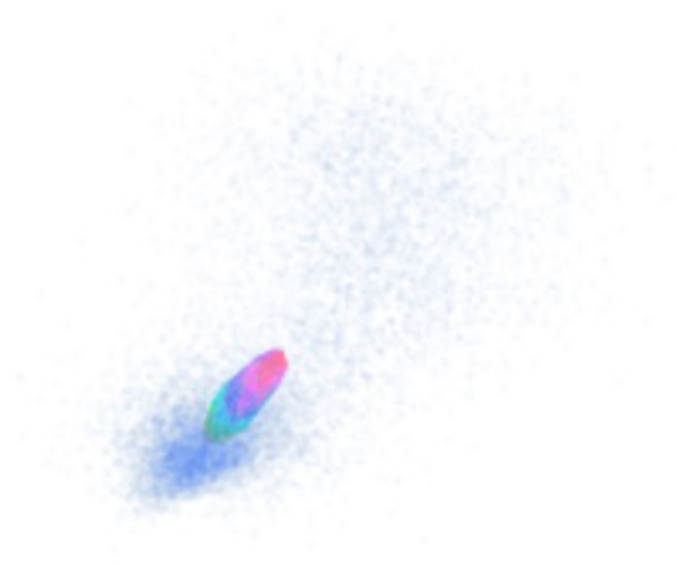

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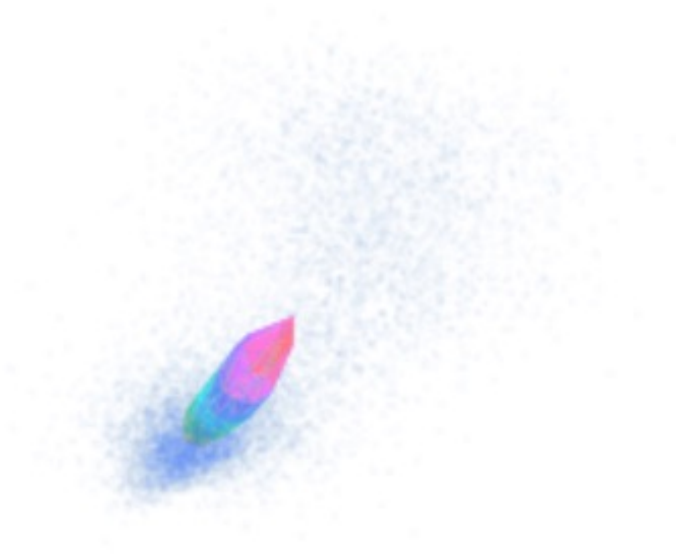

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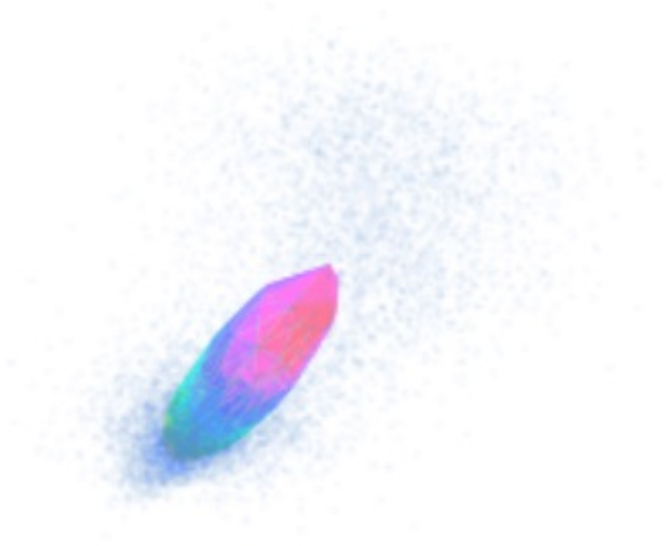

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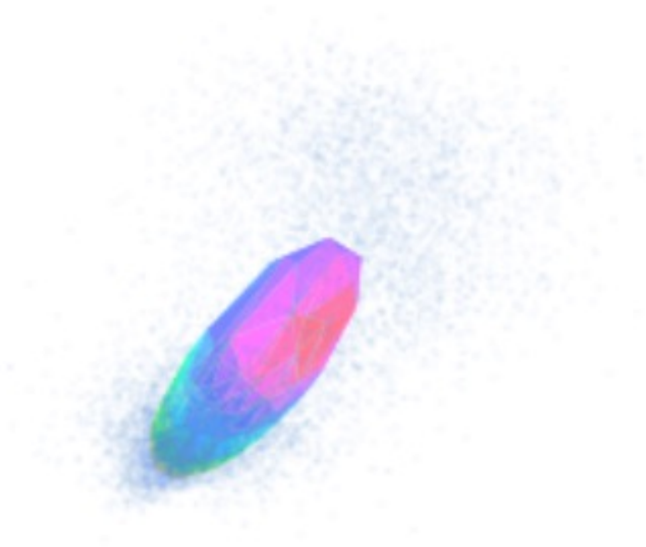

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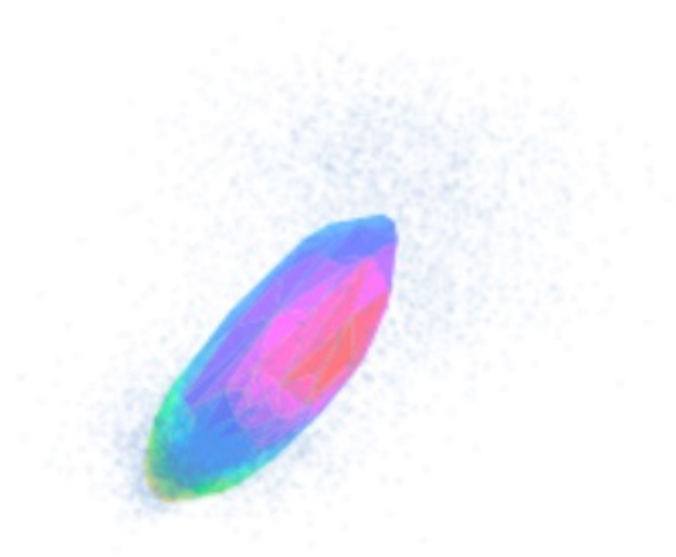

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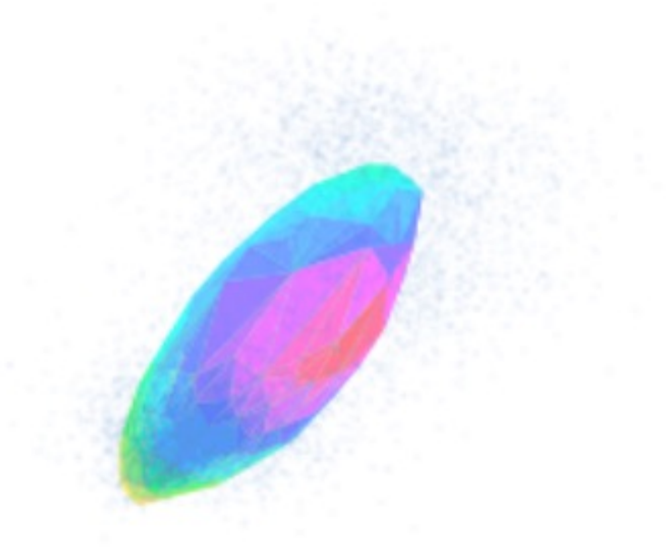

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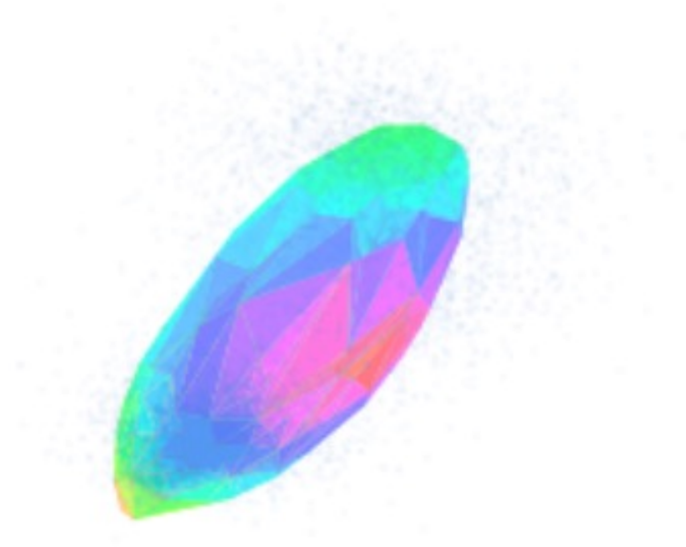

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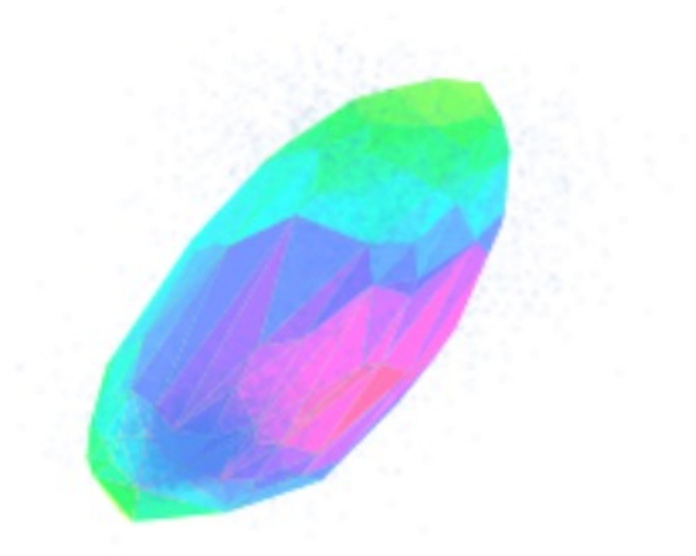

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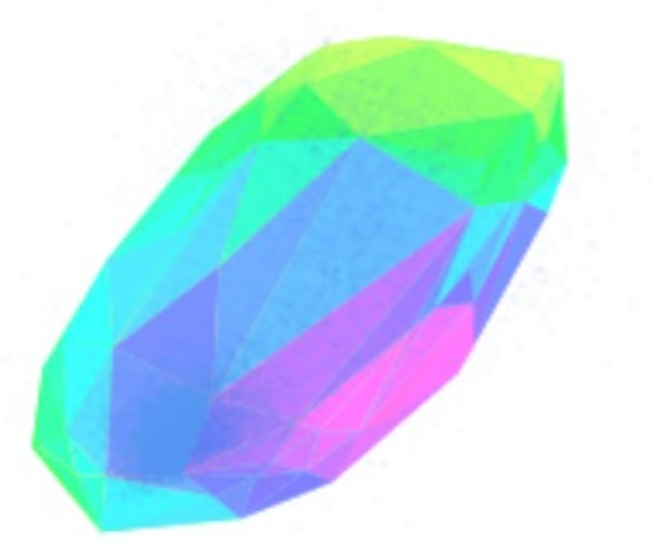
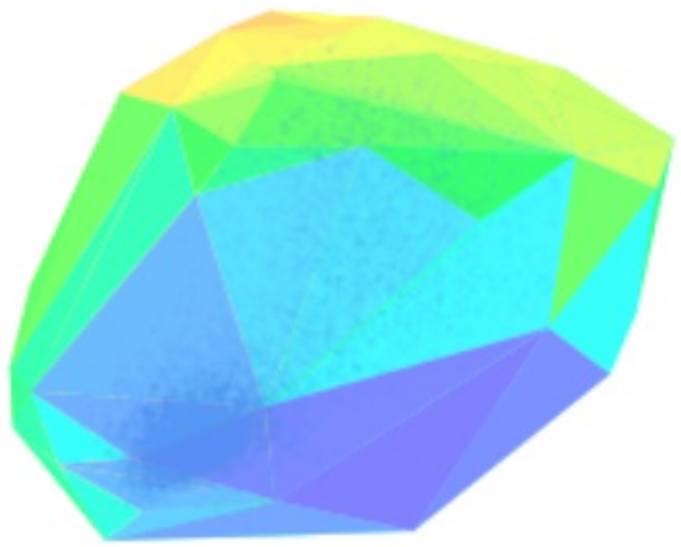
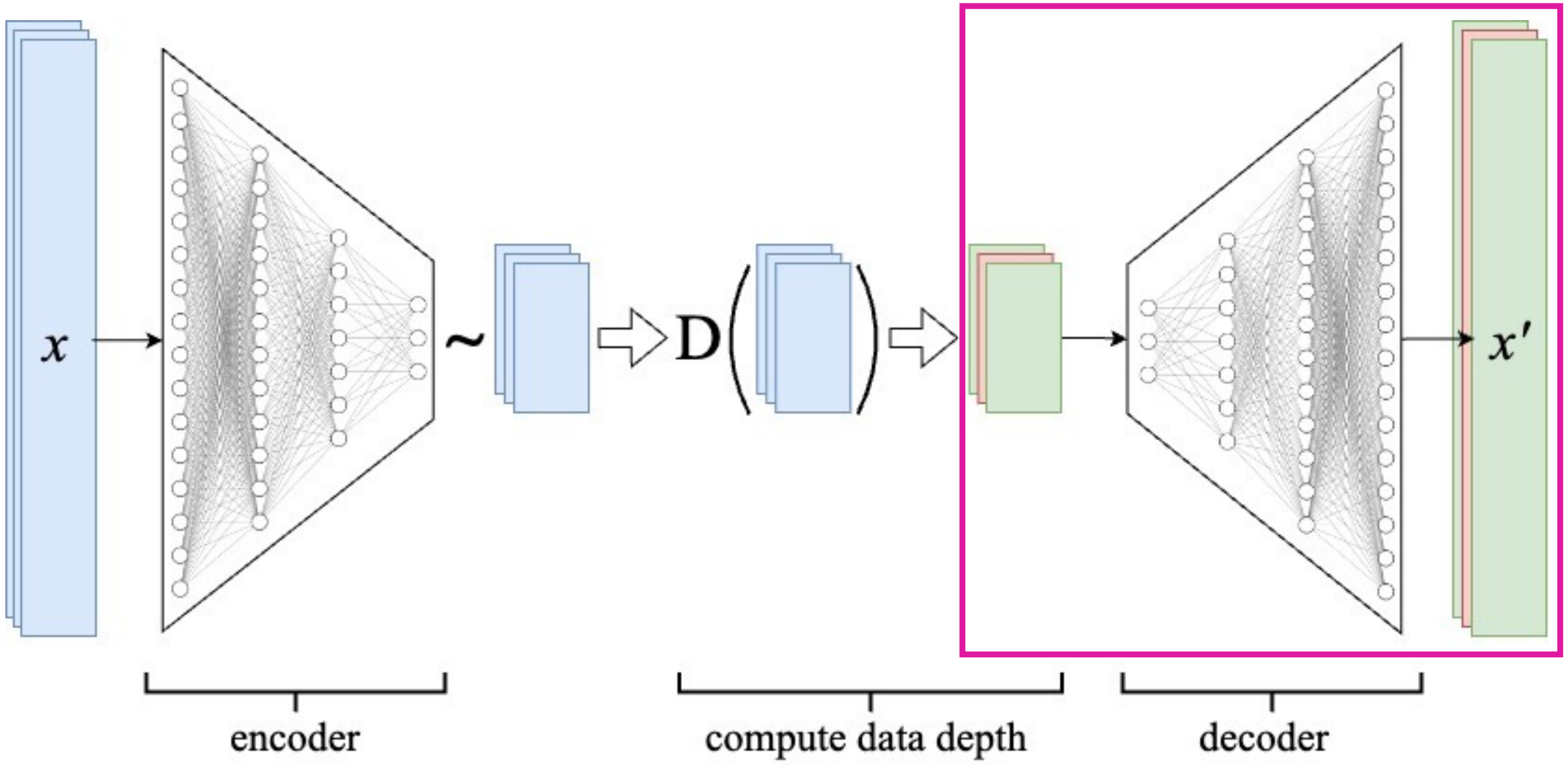


CONVEX HULL PROGRESSION

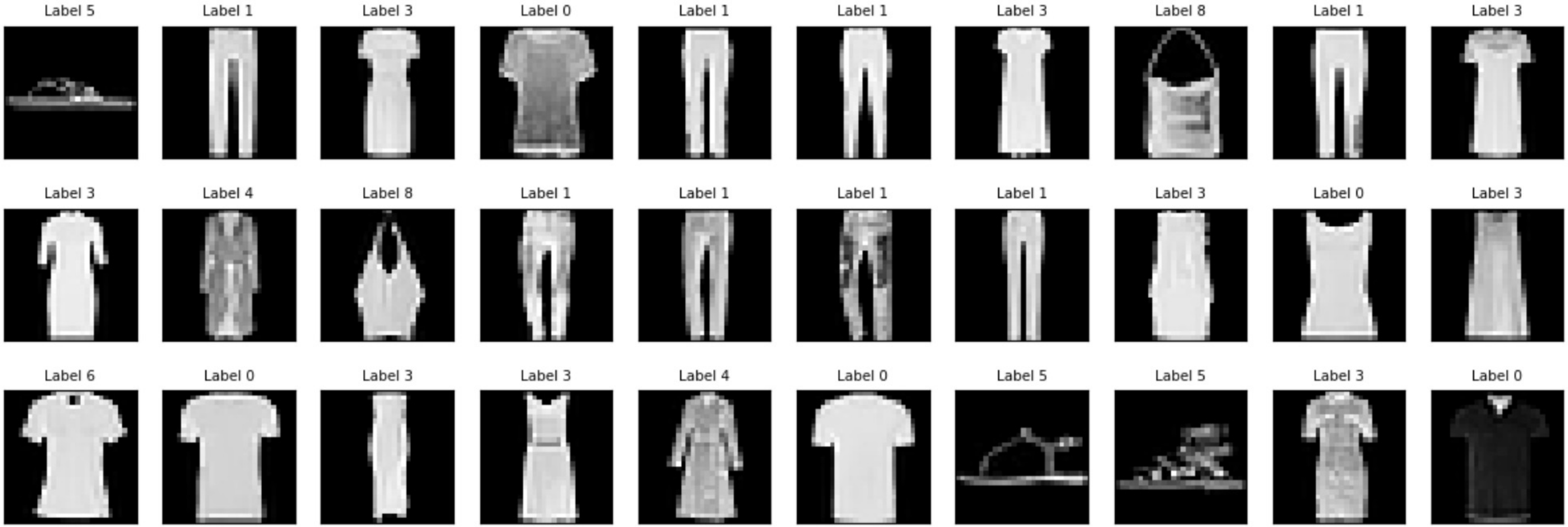


SOLUTION OVERVIEW



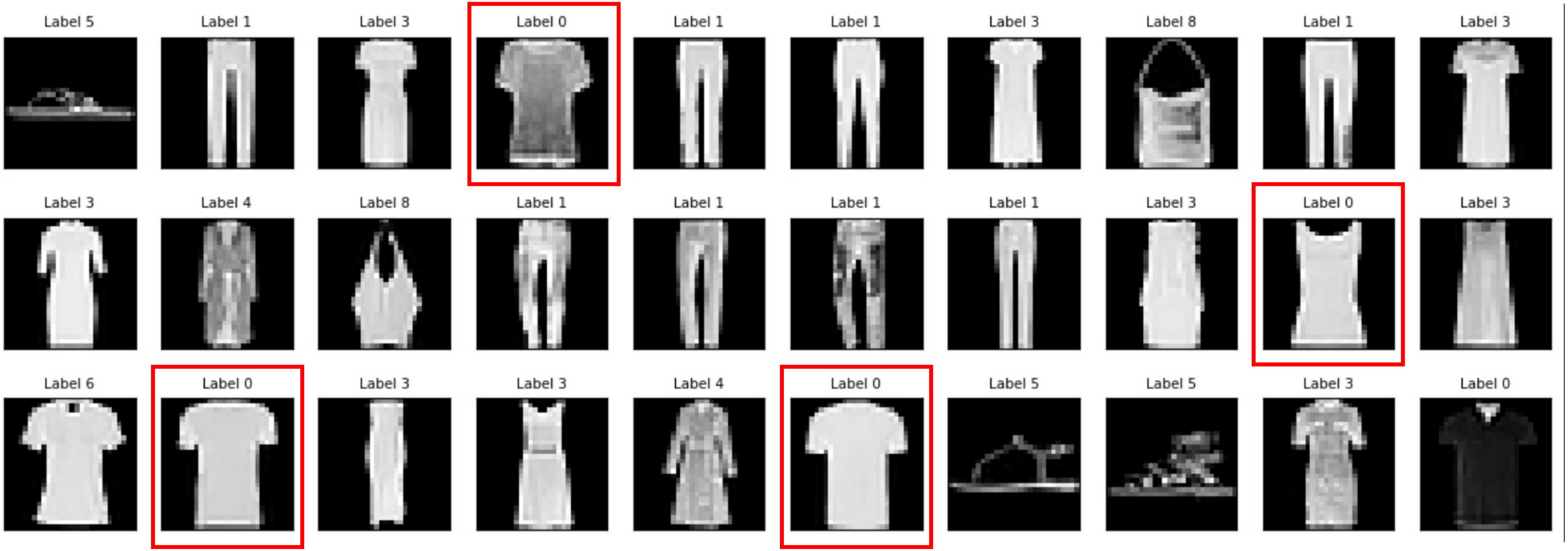
We can also use the decoder to reconstruct the images and check whether they are actually anomalies.

VISUALLY CHECKING ANOMALIES



CONCLUSION

VISUALLY CHECKING ANOMALIES



IMPROVEMENTS

- Hyperparameter Tuning
- Advanced VAE Architectures
- Regularization Techniques
- Alternative Depth Measures
- Hybrid Approaches
- Threshold Optimization
- Quantitative Evaluation
- Error Analysis
- Experiment Tracking

Q/A

APPENDIX

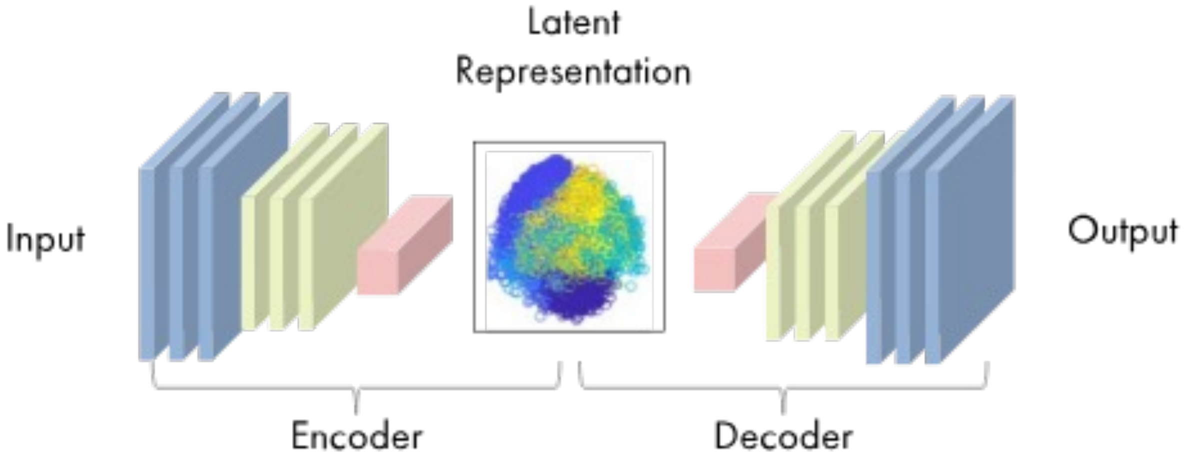
AUTOENCODERS

2 main components :

- Encoder *e(x)*: maps x to low-dimensional representation $\hat{z}$
- Decoder *d($\hat{z}$):* maps $\hat{z}$ to its original representation x

Autoencoder implements $\hat{x} = d(e(x))$

- $\hat{x}$ is the reconstruction of original input x.
- Encoder and decoder learned such that $\hat{z}$ contains as much information about x as needed to reconstruct it.



- Minimize sum of squares of differences between input and prediction: $E = \sum_i (x_i - d(e(x_i)))^2$

GITHUB REPOSITORY

- Please find all details of the implementations and the visualizations here. [https://github.com/ananya-k15/data-depth].
- In case of any issues, contact Ananya Kumar (a327kuma@uwaterloo.ca).

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