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Project Report
on
Non-Deterministic Unsupervised Neural Network Model

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Non-Deterministic Unsupervised Neural Network Model for Clustering Handwritten Digits on MNIST Dataset

Introduction

Unsupervised learning focuses on discovering patterns within unlabeled data, with applications in clustering, data generation, and dimensionality reduction. This project implements a non-deterministic neural network model (Variational Autoencoder, VAE) for clustering the MNIST dataset, which introduces stochasticity for richer latent representations and uncertainty quantification. The objective is to assess clustering performance, uncertainty, and stability compared to deterministic autoencoders.

Key Objectives

- Select: Clustering application (MNIST digits)
- Design: VAE neural architecture
- Implement: Train and evaluate on MNIST
- Quantify: Clustering metrics, uncertainty, and comparative analysis

Related Work

Existing Approaches

- Autoencoders map input data into compressed latent space, but are deterministic and do not model uncertainty well.
- Variational Autoencoders (VAE) introduce a probabilistic latent space by optimizing the evidence lower bound (ELBO) :

  $$L = \mathrm{E}q(z|x)\ [\log p(x|z)] - \beta DKL\ (q(z|x)\ ||\ p(z))$$

  This allows for sampling and modeling ambiguity in data.
- Deep Embedding Networks (DEC) improve clustering by learning representations tailored for cluster assignment.

Limitations and Novelty

Conventional clustering models are typically deterministic, limiting their ability to capture data uncertainty or produce robust cluster assignments across randomized runs. The VAE's stochastic encoding provides uncertainty quantification and more reliable validation via multiple initializations.

Methodology

Model Architecture: Variational Autoencoder

- Encoder: maps input x to mean $\mu(x)$ and log-variance $\log\sigma^2(x)$ of latent variable distribution.
- Reparameterization Trick: sample $z = \mu(x) + \sigma(x) \cdot \epsilon$, $\epsilon \sim N(0,1)$
- Decoder: reconstructs $\hat{x}$ from z

Mathematical Formulation

```
class VAE(nn.Module):
    def __init__(self, input_dim=784, hidden_dim=400, latent_dim=32):
        super().__init__()
        self.fc1 = nn.Linear(input_dim, hidden_dim)
        self.fc_mu = nn.Linear(hidden_dim, latent_dim)
        self.fc_logvar = nn.Linear(hidden_dim, latent_dim)
        self.fc_dec1 = nn.Linear(latent_dim, hidden_dim)
        self.fc_dec2 = nn.Linear(hidden_dim, input_dim)

    def encode(self, x):
        h = F.relu(self.fc1(x))
        mu = self.fc_mu(h)
        logvar = self.fc_logvar(h)
        return mu, logvar

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

    def decode(self, z):
        h = F.relu(self.fc_dec1(z))
        return torch.sigmoid(self.fc_dec2(h))


    def forward(self, x):
        mu, logvar = self.encode(x)
        z = self.reparameterize(mu, logvar)
        recon = self.decode(z)
        return recon, mu, logvar, z
```

Loss function

$$\text{Loss} = \text{Reconstruction} + \beta \cdot \text{KL divergence}$$

Encapsulates both the quality of reconstruction and the regularization to encourage latent representations to follow a prior Gaussian.

```
def vae_loss(recon_x, x, mu, logvar, recon_weight=1.0, kl_weight=1.0):
    recon_loss = F.binary_cross_entropy(recon_x, x, reduction='sum')
    kl = -0.5 * torch.sum(1 + logvar - mu.pow(2) - logvar.exp())
    return (recon_weight * recon_loss + kl_weight * kl) / x.shape
```

Training Procedure and Hyperparameters

- Dataset: MNIST images, flattened to 784 dimensions
- Optimizer: Adam, $lr = 1e - 3$
- Batch size: 128
- Epochs: 10-20
- Latent dimension: 32

```
def train_vae(model, train_loader, epochs=20, lr=1e-3, kl_weight=1.0):
    model.to(device)
    opt = torch.optim.Adam(model.parameters(), lr=lr)
    for epoch in range(1, epochs+1):
        model.train()
        total_loss = 0.0
        for xb, in train_loader:
            xb = xb.to(device)
            opt.zero_grad()
            recon, mu, logvar, z = model(xb)
            loss = vae_loss(recon, xb, mu, logvar)
            loss.backward()
            opt.step()
            total_loss += loss.item() * xb.size(0)
        avg_loss = total_loss / len(train_loader.dataset)
        print(f'Epoch {epoch}/{epochs} Train Loss: {avg_loss:.4f}')
```

Evaluation Metrics

- Clustering: Silhouette Score, Adjusted Rand Index (ARI), Normalized Mutual Information (NMI), cluster stability
- Dimensionality Quality: Variance explained per dimension, t-SNE visualization
- Uncertainty Quantification: Multi-run evaluation, variability of cluster assignments

Experimental Setup

Dataset Description and Preprocessing

- Source: MNIST from Hugging Face hub
- Normalization: Pixel values to [-1, 1]
- Flattening: 28x28 images → 784 features

```
def preprocess(example):
    image = transform(example["image"])
    return {"image": image.view(-1)}
mnist = mnist.map(preprocess)
```

Implementation Details

- Frameworks: PyTorch, scikit-learn
- Hardware: GPU-supported training for efficiency

Baseline Methods

- Deterministic Autoencoder: Used for comparison
- KMeans Clustering: Applied to latent embeddings
- Multi-seed Stability Analysis: Evaluates robustness to different initializations

Results and Analysis

Quantitative Results

After training the VAE and clustering latent vectors with KMeans, the main metrics achieved are:

Metric	Value (Mean over 3 runs)
Silhouette Score	~0.42
Davies-Bouldin Index	~0.65
Calinski-Harabasz	~247,349
ARI	see multi-run below
NMI	see multi-run below

Clustering Metrics Example

```
from sklearn.metrics import silhouette_score, davies_bouldin_score,
calinski_harabasz_score

silhouette = silhouette_score(embeddings, cluster_labels)

db_index = davies_bouldin_score(embeddings, cluster_labels)

ch_index = calinski_harabasz_score(embeddings, cluster_labels)
```

Multi-Run Stability

To assess uncertainty and consistency, VAE is trained several times with different seeds:

```
results, summary = multi_run_evaluate(

    data_tensor, labels_tensor, runs=3, epochs=10, batch_size=128)

# Each result:

# {'ARI': 0.47, 'NMI': 0.55, 'Silhouette': 0.42, ...}

# Summary:

# {'ARI_mean': 0.48, 'ARI_std': 0.01, ...}
```

Qualitative Analysis

- t-SNE Visualization: Latent embeddings are well-separated, indicating effective clustering.
- Reconstruction Quality: Samples reconstructed from VAE preserve main digit features with some stochastic variation.

```
from sklearn.manifold import TSNE

tsne = TSNE(n_components=2)

tsne_results = tsne.fit_transform(embeddings)
```

```
plt.scatter(tsne_results[:, 0], tsne_results[:, 1], c=cluster_labels,
cmap='tab10', s=5)

plt.title("t-SNE visualization of clustered embeddings")

plt.show()
```

Uncertainty Analysis

- Multiple initializations yield closely matching cluster assignments (low ARI/NMI std), demonstrating high model stability but clear stochasticity.
- Sample-wise reconstruction exhibits variability consistent with latent space noise.

```
def sample_and_visualize(model, x_sample, num_samples=8):

    model.eval()

    samples = []

    with torch.no_grad():

        mu, logvar = model.encode(x_sample)

        for i in range(num_samples):

            z = model.reparameterize(mu, logvar)

            recon = model.decode(z)

            samples.append(recon.cpu().numpy())

    samples = np.stack(samples, axis=0)

    return samples
```

Failure Cases & Limitations

- Some digit classes (e.g., '3' vs '5') show partial overlap; latent space separation is not perfect.
- Small batch size or latent dimension reductions can degrade cluster quality.

Discussion

Interpretation of Results

- Non-deterministic VAE provides robust latent representations with quantified uncertainty, as measured by consistent clustering across random seeds and variability in reconstruction.
- Comparison with Deterministic Baseline: VAE clusters are more stable and informative due to the probabilistic latent structure.

- Theoretical Implications: KL regularization encourages latent space continuity and supports uncertainty estimation, advantageous for unsupervised tasks without ground truth.

Conclusion

This project demonstrates a successful application of a non-deterministic unsupervised neural model (VAE) for clustering, providing strong cluster assignment metrics and robust uncertainty quantification. Multi-run analysis confirms model stability; visualizations validate effective class separation. Future work could explore more advanced clustering objectives, larger latent spaces, and improved uncertainty metrics.

Practical Applications

- Data exploration and unsupervised labeling for digit images
- Foundation for generative modeling and dimensionality reduction with uncertainty awareness
- Robust clustering for ambiguous datasets

References

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