

▼ VQ-VAE by Aäron van den Oord et al. in PyTorch

Introduction

Variational Auto Encoders (VAEs) can be thought of as what all but the last layer of a neural network is doing, namely feature extraction or separating out the data. Thus given some data we can think of using a neural network for representation generation.

Recall that the goal of a generative model is to estimate the probability distribution of high dimensional data such as images, videos, audio or even text by learning the underlying structure in the data as well as the dependencies between the different elements of the data. This is very useful since we can then use this representation to generate new data with similar properties. This way we can also learn useful features from the data in an unsupervised fashion.

The VQ-VAE uses a discrete latent representation mostly because many important real-world objects are discrete. For example in images we might have categories like "Cat", "Car", etc. and it might not make sense to interpolate between these categories. Discrete representations are also easier to model since each category has a single value whereas if we had a continuous latent space then we will need to normalize this density function and learn the dependencies between the different variables which could be very complex.

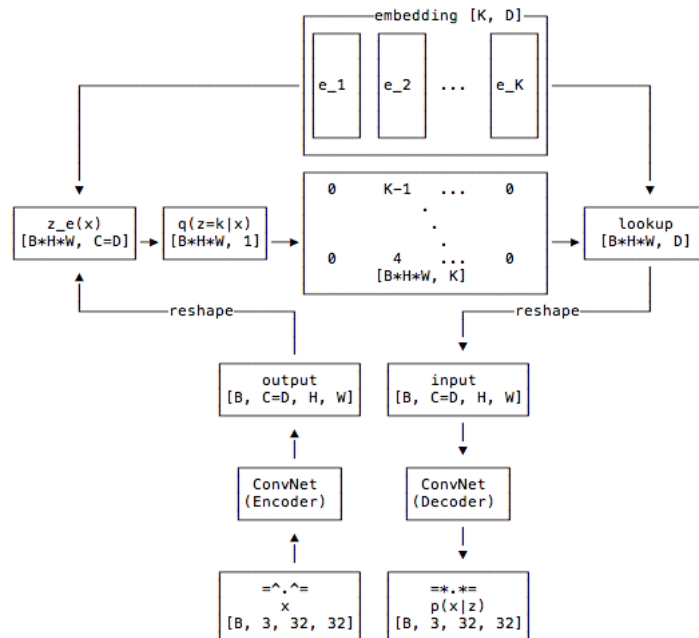
Code

I have followed the code from the TensorFlow implementation by the author which you can find here [vqvae.py](#) and [vqvae_example.ipynb](#).

Another PyTorch implementation is found at [pytorch-vqvae](#).

Basic Idea

The overall architecture is summarized in the diagram below:



We start by defining a latent embedding space of dimension $[K, D]$ where K are the number of embeddings and D is the dimensionality of each latent embedding vector, i.e. $e_i \in \mathbb{R}^D$. The model is comprised of an encoder and a decoder. The encoder will map the input to a sequence of discrete latent variables, whereas the decoder will try to reconstruct the input from these latent sequences.

More precisely, the model will take in batches of RGB images, say x , each of size 32×32 for our example, and pass it through a ConvNet encoder producing some output $E(x)$, where we make sure the channels are the same as the dimensionality of the latent embedding vectors. To calculate the discrete latent variable we find the nearest embedding vector and output its index.

The input to the decoder is the embedding vector corresponding to the index which is passed through the decoder to produce the reconstructed image.

Since the nearest neighbour lookup has no real gradient in the backward pass we simply pass the gradients from the decoder to the encoder unaltered. The intuition is that since the output representation of the encoder and the input to the decoder share the same D channel dimensional space, the gradients contain useful information for how the encoder has to change its output to lower the reconstruction loss.

▼ Loss

The total loss is actually composed of three components

1. **reconstruction loss**: which optimizes the decoder and encoder
2. **codebook loss**: due to the fact that gradients bypass the embedding, we use a dictionary learning algorithm which uses an l_2 error to move the embedding vectors e_i towards the encoder output
3. **commitment loss**: since the volume of the embedding space is dimensionless, it can grow arbitrarily if the embeddings e_i do not train as fast as the encoder parameters, and thus we add a commitment loss to make sure that the encoder commits to an embedding

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1 !pip install umap-learn
```

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  Downloading umap-learn-0.5.4.tar.gz (90 kB)
    ----- 90.8/90.8 kB 2.3 MB/s eta 0:00:00
  Preparing metadata (setup.py) ... done
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  Preparing metadata (setup.py) ... done
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  Building wheel for umap-learn (setup.py) ... done
  Created wheel for umap-learn: filename=umap_learn-0.5.4-py3-none-any.whl size=86770 sha256=028e0b5ca888e0ee4255c51a480059a1f16835bba74
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  Stored in directory: /root/.cache/pip/wheels/4a/38/5d/f60a40a66a9512b7e5e83517ebc2d1b42d857be97d135f1096
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Installing collected packages: pynndescent, umap-learn
Successfully installed pynndescent-0.5.10 umap-learn-0.5.4
```

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1 from __future__ import print_function
2
3
4 import matplotlib.pyplot as plt
5 import numpy as np
6 from scipy.signal import savgol_filter
7
8
9 from six.moves import xrange
10
11 import umap
12
13 import torch
14 import torch.nn as nn
15 import torch.nn.functional as F
16 from torch.utils.data import DataLoader
17 import torch.optim as optim
18
19 import torchvision.datasets as datasets
20 import torchvision.transforms as transforms
21 from torchvision.utils import make_grid
```

```
1 device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
```

▼ Load Data

```
1 training_data = datasets.CIFAR10(root="data", train=True, download=True,
2                                  transform=transforms.Compose([
3                                      transforms.ToTensor(),
4                                      transforms.Normalize((0.5,0.5,0.5), (1.0,1.0,1.0))
5                                  ]))
```

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5         ]))
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7 validation_data = datasets.CIFAR10(root="data", train=False, download=True,
8                                   transform=transforms.Compose([
9                                       transforms.ToTensor(),
10                                      transforms.Normalize((0.5,0.5,0.5), (1.0,1.0,1.0))
11                                      ]))
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13 Downloading https://www.cs.toronto.edu/~kriz/cifar-10-python.tar.gz to data/cifar-10-python.tar.gz
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```

We will also implement a slightly modified version which will use exponential moving averages to update the embedding vectors instead of an auxiliary loss. This has the advantage that the embedding updates are independent of the choice of optimizer for the encoder, decoder and other parts of the architecture. For most experiments the EMA version trains faster than the non-EMA version.

```

1  class VectorQuantizerEMA(nn.Module):
2      def __init__(self, num_embeddings, embedding_dim, commitment_cost, decay, epsilon=1e-5):
3          super(VectorQuantizerEMA, self).__init__()
4
5          self._embedding_dim = embedding_dim
6          self._num_embeddings = num_embeddings
7
8          self._embedding = nn.Embedding(self._num_embeddings, self._embedding_dim)
9          self._embedding.weight.data.normal_()
10         self._commitment_cost = commitment_cost
11
12         self.register_buffer('_ema_cluster_size', torch.zeros(num_embeddings))
13         self._ema_w = nn.Parameter(torch.Tensor(num_embeddings, self._embedding_dim))
14         self._ema_w.data.normal_()
15
16         self._decay = decay
17         self._epsilon = epsilon
18
19     def forward(self, inputs):
20         # convert inputs from BCHW -> BHWC
21         inputs = inputs.permute(0, 2, 3, 1).contiguous()
22         input_shape = inputs.shape
23
24         # Flatten input
25         flat_input = inputs.view(-1, self._embedding_dim)
26
27         # Calculate distances
28         distances = (torch.sum(flat_input**2, dim=1, keepdim=True)
29                     + torch.sum(self._embedding.weight**2, dim=1)
30                     - 2 * torch.matmul(flat_input, self._embedding.weight.t()))
31
32         # Encoding
33         encoding_indices = torch.argmax(distances, dim=1).unsqueeze(1)
34         encodings = torch.zeros(encoding_indices.shape[0], self._num_embeddings, device=inputs.device)
35         encodings.scatter_(1, encoding_indices, 1)
36
37         # Quantize and unflatten
38         quantized = torch.matmul(encodings, self._embedding.weight).view(input_shape)
39
40         # Use EMA to update the embedding vectors
41         if self.training:
42             self._ema_cluster_size = self._ema_cluster_size * self._decay + \
43                                     (1 - self._decay) * torch.sum(encodings, 0)
44
45             # Laplace smoothing of the cluster size
46             n = torch.sum(self._ema_cluster_size.data)
47             self._ema_cluster_size = (
48                 (self._ema_cluster_size + self._epsilon)
49                 / (n + self._num_embeddings * self._epsilon) * n)
50
51             dw = torch.matmul(encodings.t(), flat_input)
52             self._ema_w = nn.Parameter(self._ema_w * self._decay + (1 - self._decay) * dw)
53
54             self._embedding.weight = nn.Parameter(self._ema_w / self._ema_cluster_size.unsqueeze(1))
55
56         # Loss
57         e_latent_loss = F.mse_loss(quantized.detach(), inputs)
58         loss = self._commitment_cost * e_latent_loss
59
60         # Straight Through Estimator
61         quantized = inputs + (quantized - inputs).detach()
62         avg_probs = torch.mean(encodings, dim=0)
63         perplexity = torch.exp(-torch.sum(avg_probs * torch.log(avg_probs + 1e-10)))
64
65         # convert quantized from BHWC -> BCHW
66         return loss, quantized.permute(0, 3, 1, 2).contiguous(), perplexity, encodings

```

▼ Encoder & Decoder Architecture

The encoder and decoder architecture is based on a ResNet and is implemented below:

```

1 class Residual(nn.Module):
2     def __init__(self, in_channels, num_hiddens, num_residual_hiddens):
3         super(Residual, self).__init__()
4         self._block = nn.Sequential(
5             nn.ReLU(True),
6             nn.Conv2d(in_channels=in_channels,
7                       out_channels=num_residual_hiddens,
8                       kernel_size=3, stride=1, padding=1, bias=False),
9             nn.ReLU(True),
10            nn.Conv2d(in_channels=num_residual_hiddens,
11                     out_channels=num_hiddens,
12                     kernel_size=1, stride=1, bias=False)
13        )
14
15    def forward(self, x):
16        return x + self._block(x)
17
18
19 class ResidualStack(nn.Module):
20     def __init__(self, in_channels, num_hiddens, num_residual_layers, num_residual_hiddens):
21         super(ResidualStack, self).__init__()
22         self._num_residual_layers = num_residual_layers
23         self._layers = nn.ModuleList([Residual(in_channels, num_hiddens, num_residual_hiddens)
24                                         for _ in range(self._num_residual_layers)])
25
26    def forward(self, x):
27        for i in range(self._num_residual_layers):
28            x = self._layers[i](x)
29        return F.relu(x)
30
31
32 class Encoder(nn.Module):
33     def __init__(self, in_channels, num_hiddens, num_residual_layers, num_residual_hiddens):
34         super(Encoder, self).__init__()
35
36         self._conv_1 = nn.Conv2d(in_channels=in_channels,
37                                   out_channels=num_hiddens//2,
38                                   kernel_size=4,
39                                   stride=2, padding=1)
40
41         self._conv_2 = nn.Conv2d(in_channels=num_hiddens//2,
42                                   out_channels=num_hiddens,
43                                   kernel_size=4,
44                                   stride=2, padding=1)
45
46         self._conv_3 = nn.Conv2d(in_channels=num_hiddens,
47                                   out_channels=num_hiddens,
48                                   kernel_size=3,
49                                   stride=1, padding=1)
50
51         self._residual_stack = ResidualStack(in_channels=num_hiddens,
52                                               num_hiddens=num_hiddens,
53                                               num_residual_layers=num_residual_layers,
54                                               num_residual_hiddens=num_residual_hiddens)
55
56    def forward(self, inputs):
57        x = self._conv_1(inputs)
58        x = F.relu(x)
59
60        x = self._conv_2(x)
61        x = F.relu(x)
62
63        x = self._conv_3(x)
64        return self._residual_stack(x)
65
66
67 class Decoder(nn.Module):
68     def __init__(self, in_channels, num_hiddens, num_residual_layers, num_residual_hiddens):
69         super(Decoder, self).__init__()
70
71         self._conv_1 = nn.Conv2d(in_channels=in_channels,
72                                   out_channels=num_hiddens,
73                                   kernel_size=3,
74                                   stride=1, padding=1)
75
76         self._residual_stack = ResidualStack(in_channels=num_hiddens,
77                                               num_hiddens=num_hiddens,
78                                               num_residual_layers=num_residual_layers,

```

```

13             num_residual_hiddens=num_residual_hiddens)
14
15         self._conv_trans_1 = nn.ConvTranspose2d(in_channels=num_hiddens,
16                                                  out_channels=num_hiddens//2,
17                                                  kernel_size=4,
18                                                  stride=2, padding=1)
19
20         self._conv_trans_2 = nn.ConvTranspose2d(in_channels=num_hiddens//2,
21                                                  out_channels=3,
22                                                  kernel_size=4,
23                                                  stride=2, padding=1)
24
25     def forward(self, inputs):
26         x = self._conv_1(inputs)
27
28         x = self._residual_stack(x)
29
30         x = self._conv_trans_1(x)
31         x = F.relu(x)
32
33         return self._conv_trans_2(x)

```

▼ Train

We use the hyperparameters from the author's code:

```

1 batch_size = 256
2 num_training_updates = 200000
3
4 num_hiddens = 128
5 num_residual_hiddens = 32
6 num_residual_layers = 2
7
8 embedding_dim = 64
9 num_embeddings = 512
10
11 commitment_cost = 0.25
12
13 decay = 0
14
15 learning_rate = 1e-4

1 training_loader = DataLoader(training_data,
2                               batch_size=batch_size,
3                               shuffle=True,
4                               pin_memory=True)

1 validation_loader = DataLoader(validation_data,
2                                 batch_size=32,
3                                 shuffle=False,
4                                 pin_memory=True)

1 class Model(nn.Module):
2     def __init__(self, num_hiddens, num_residual_layers, num_residual_hiddens,
3                 num_embeddings, embedding_dim, commitment_cost, decay=0):
4         super(Model, self).__init__()
5
6         self._encoder = Encoder(3, num_hiddens,
7                                 num_residual_layers,
8                                 num_residual_hiddens)
9         self._pre_vq_conv = nn.Conv2d(in_channels=num_hiddens,
10                                       out_channels=embedding_dim,
11                                       kernel_size=1,
12                                       stride=1)
13         if decay > 0.0:
14             self._vq_vae = VectorQuantizerEMA(num_embeddings, embedding_dim,
15                                                commitment_cost, decay)
16         else:
17             self._vq_vae = VectorQuantizer(num_embeddings, embedding_dim,
18                                             commitment_cost)
19         self._decoder = Decoder(embedding_dim,
20                                 num_hiddens,
21                                 num_residual_layers,

```

```

22             num_residual_hiddens)
23
24     def forward(self, x):
25         z = self._encoder(x)
26         z = self._pre_vq_conv(z)
27         loss, quantized, perplexity, _ = self._vq_vae(z)
28         x_recon = self._decoder(quantized)
29
30         return loss, x_recon, perplexity

1 model = Model(num_hiddens, num_residual_layers, num_residual_hiddens,
2               num_embeddings, embedding_dim,
3               commitment_cost, decay).to(device)

1 optimizer = optim.Adam(model.parameters(), lr=learning_rate, amsgrad=False)

1 model.train()
2 train_res_recon_error = []
3 train_res_perplexity = []
4
5 for i in xrange(num_training_updates):
6     (data, _) = next(iter(training_loader))
7     data = data.to(device)
8     optimizer.zero_grad()
9
10    vq_loss, data_recon, perplexity = model(data)
11    recon_error = F.mse_loss(data_recon, data) / data_variance
12    loss = recon_error + vq_loss
13    loss.backward()
14
15    optimizer.step()
16
17    train_res_recon_error.append(recon_error.item())
18    train_res_perplexity.append(perplexity.item())
19
20    if (i+1) % 100 == 0:
21        print('%d iterations' % (i+1))
22        print('recon_error: %.3f' % np.mean(train_res_recon_error[-100:]))
23        print('perplexity: %.3f' % np.mean(train_res_perplexity[-100:]))
24        print()

```



```
199600 iterations
recon_error: 0.053
perplexity: 253.702
```

```
199700 iterations
recon_error: 0.053
perplexity: 253.880
```

```
199800 iterations
recon_error: 0.053
perplexity: 253.689
```

```
199900 iterations
recon_error: 0.053
perplexity: 254.936
```

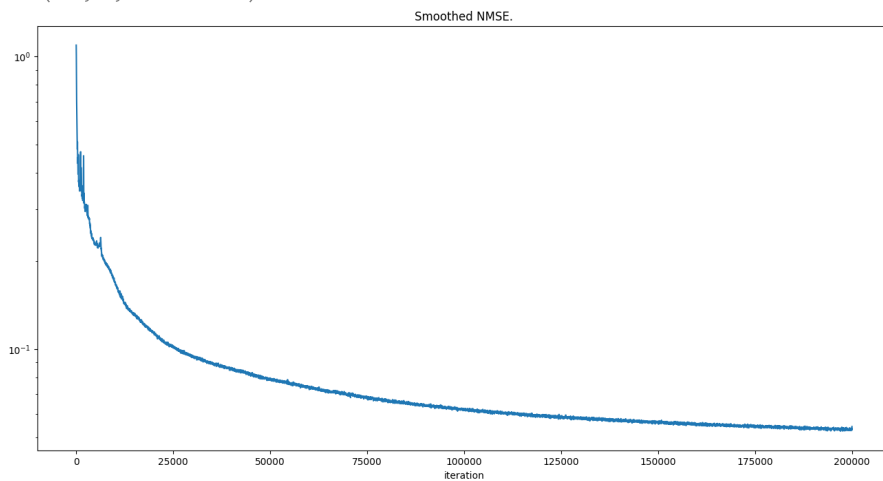
```
200000 iterations
recon_error: 0.053
perplexity: 254.751
```

▼ Plot Loss

```
1 train_res_recon_error_smooth = savgol_filter(train_res_recon_error, 201, 7)
2 train_res_perplexity_smooth = savgol_filter(train_res_perplexity, 201, 7)
```

```
1 f = plt.figure(figsize=(16,8))
2 ax = f.add_subplot(1,1,1)
3 ax.plot(train_res_recon_error_smooth)
4 ax.set_yscale('log')
5 ax.set_title('Smoothed NMSE.')
6 ax.set_xlabel('iteration')
```

```
Text(0.5, 0, 'iteration')
```



▼ View Reconstructions

```
1 model.eval()
2
3 (valid_originals, _) = next(iter(validation_loader))
4 valid_originals = valid_originals.to(device)
5
6 vq_output_eval = model._pre_vq_conv(model._encoder(valid_originals))
7 _, valid_quantize, _, _ = model._vq_vae(vq_output_eval)
8 valid_reconstructions = model._decoder(valid_quantize)
```



```

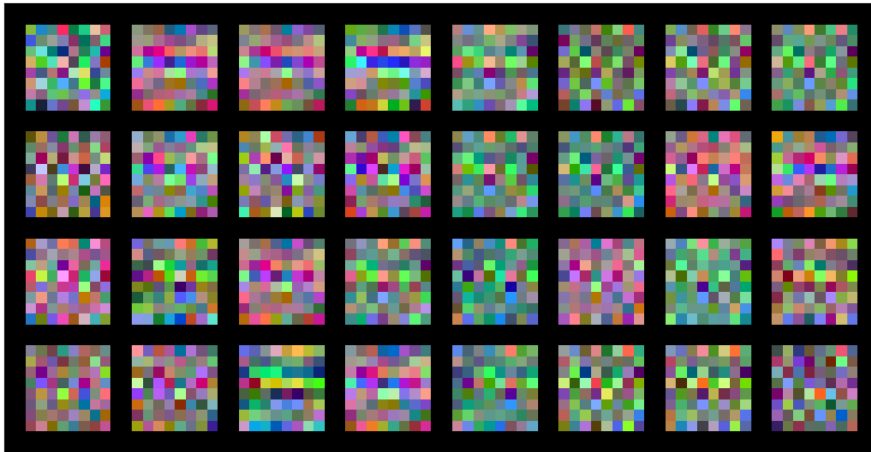
1 (train_originals, _) = next(iter(training_loader))
2 train_originals = train_originals.to(device)
3 _, train_reconstructions, _, _ = model._vq_vae(train_originals)

1 plt.rcParams["figure.figsize"] = (10,8)

1 def show(img):
2     npimg = img.numpy()
3     fig = plt.imshow(np.transpose(npimg, (1,2,0)), interpolation='nearest')
4     fig.axes.get_xaxis().set_visible(False)
5     fig.axes.get_yaxis().set_visible(False)

1 # Latent space images
2 latents = valid_quantize.view(32 * 64, embedding_dim)
3 U, S, V = torch.pca_lowrank(latents)
4 projections = torch.matmul(latents, V[:, :3]).view(32, 3, 8, 8) # project to 3 channel to view the latents as RGB images
5 latent_imgs = projections.cpu().data
6 for i in range(len(latent_imgs)):
7     for j in range(3):
8         tmp = latent_imgs[i,j,:,:]
9         tmp -= tmp.min()
10        tmp /= tmp.max()
11        latent_imgs[i,j,:,:] = tmp
12 show(make_grid(latent_imgs), )

```

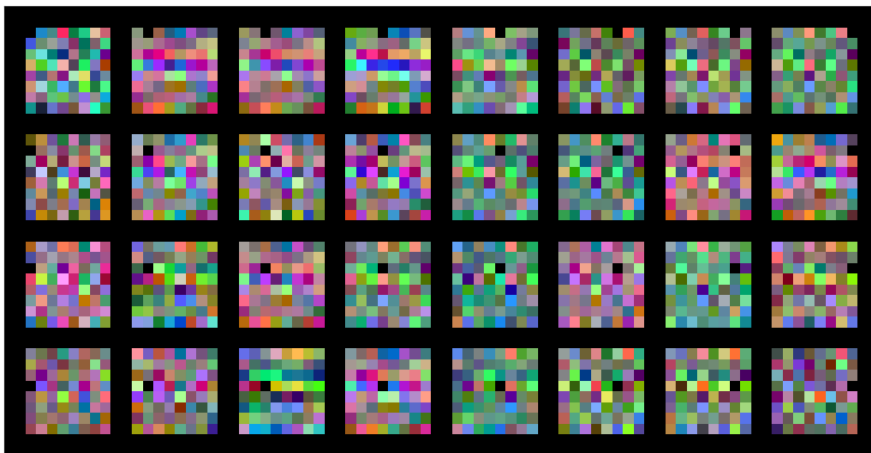


```

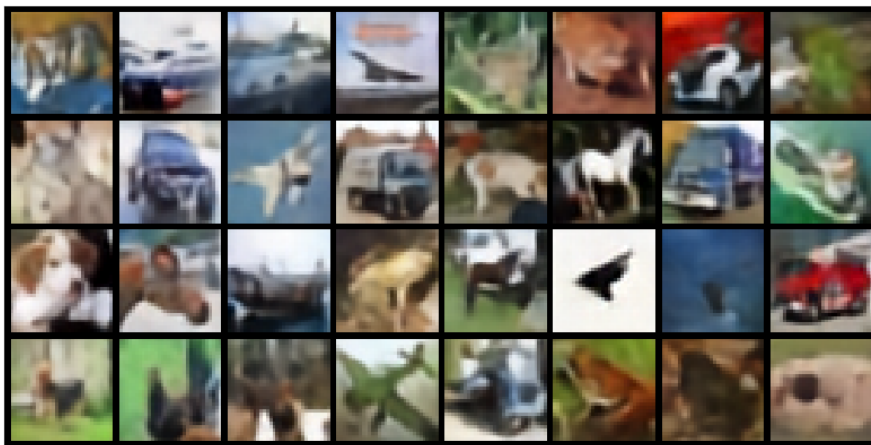
1 # create masks
2 masks = torch.ones((32, 3, 8, 8))
3 for i, mask in enumerate(masks):
4     mask[:, i // 8, i % 8] = 0
5 show(make_grid(masks), )

```

```
1 masked_latent_imgs = torch.mul(masks, latent_imgs)
2 show(make_grid(masked_latent_imgs), )
```

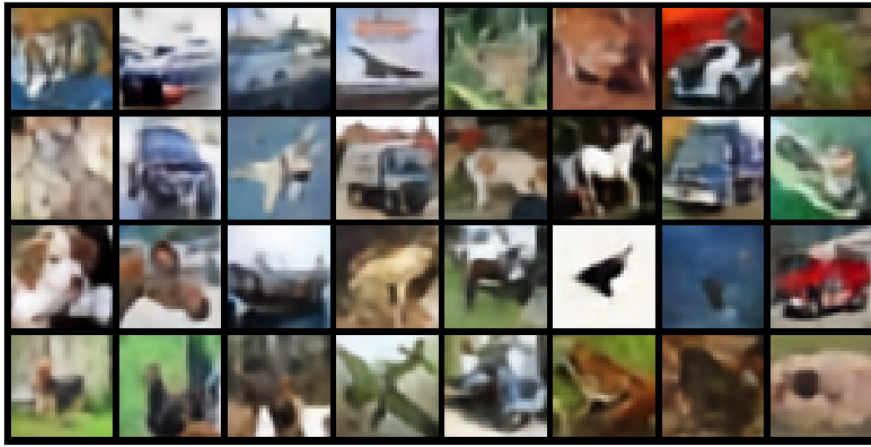


```
1 reconstructed_imgs = valid_reconstructions.cpu().data + 0.5
2
3 for i in range(len(reconstructed_imgs)):
4     for j in range(3):
5         tmp = torch.clamp(reconstructed_imgs[i,j,:,:), 0, 1)
6         reconstructed_imgs[i,j,:,:) = tmp
7 show(make_grid(reconstructed_imgs), )
```

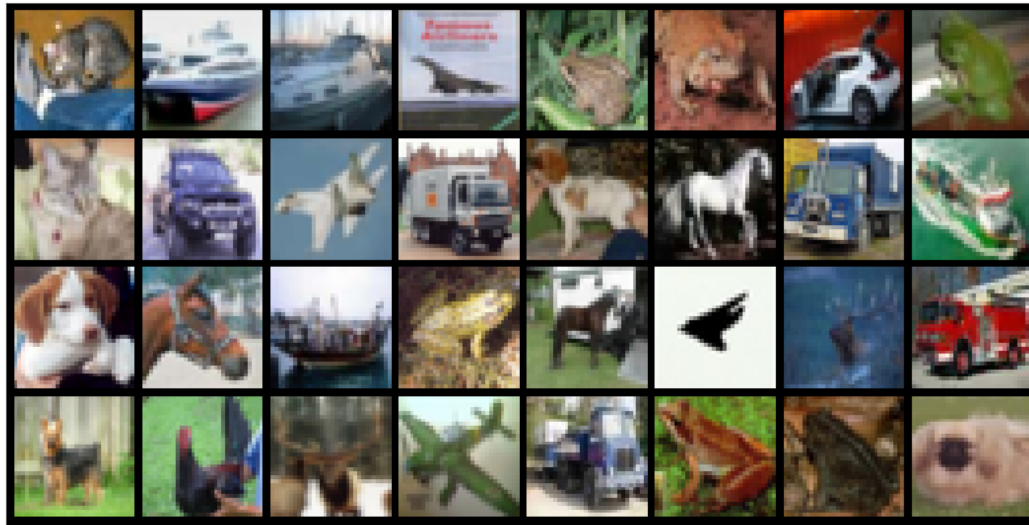


```
1 masks = torch.ones((32, embedding_dim, 8, 8))
2 for i, mask in enumerate(masks):
3     mask[:, i // 8, i % 8] = 0
4 masked_latent_imgs = torch.mul(masks.cuda(), latents.view(32, embedding_dim, 8, 8))
5 masked_valid_reconstructions = model._decoder(masked_latent_imgs)

1 for i in range(len(masked_valid_reconstructions)):
2     for j in range(3):
3         tmp = torch.clamp(masked_valid_reconstructions[i,j,:,:) + 0.5, 0, 1)
4         masked_valid_reconstructions[i,j,:,:) = tmp
5 show(make_grid(masked_valid_reconstructions.cpu().data), )
```



```
1 show(make_grid(valid_originals.cpu()+0.5))
```



▼ View Embedding

```
1 proj = umap.UMAP(n_neighbors=3,
2                   min_dist=0.1,
3                   metric='cosine').fit_transform(model._vq_vae._embedding.weight.data.cpu())

1 plt.scatter(proj[:,0], proj[:,1], alpha=0.3)
```

