Project - Stable Diffusion

Team Members:

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Problem Statement:

The project focuses on pre-training a Stable Diffusion model from scratch to generate conditional color images based on inputs such as numbers, classes, tokens, or text. Using the U-Net architecture with skip connections, the model will learn to iteratively denoise noisy samples, transforming random noise into meaningful images.

The goal is to adapt and train the model on a selected color image dataset entirely in PyTorch, using the provided codebase without relying on pre-trained weights, fine-tuning, or external frameworks. Challenges include implementing the diffusion process, designing a custom loss function to predict and remove noise effectively, and ensuring the generated images are accurate and high-quality based on the given conditions. This project will deepen the understanding of training diffusion models from scratch while demonstrating their generative capabilities.

Dataset: (https://www.cs.toronto.edu/~kriz/cifar.html)

The CIFAR-10 and CIFAR-100 datasets are popular benchmarks in machine learning and computer vision, featuring 32x32 color images for tasks like classification and generation.

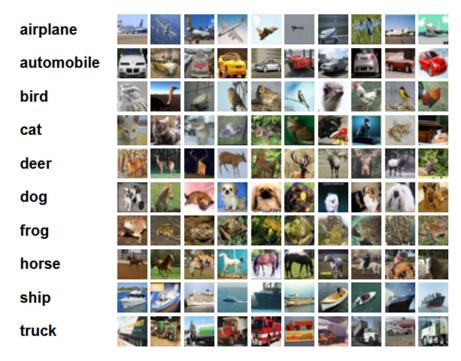
Dataset Overview:

CIFAR-10: 60,000 images (32x32 color) across 10 classes (e.g., airplane, car, dog). Divided into 50,000 training images and 10,000 testing images.

CIFAR-100: 60,000 images (32x32 color) across 100 classes, grouped into 20 superclasses. Each image has a "fine" (specific) and "coarse" (group) label.

The CIFAR-10 and CIFAR-100 datasets are well-suited for this project due to their manageable size, diverse classes, and efficient 32x32 color images, ideal for training a Stable Diffusion model from scratch. Their variety of objects, animals, and scenes provides rich visual features for the model to learn, while the class labels serve as conditions for generating specific images, such as "dog" or "airplane" in CIFAR-10 or more detailed classes like "tulip" in CIFAR-100.

These datasets align with the project's goals of generating conditional color images. Their small resolution enables efficient training and quick iterations, making them practical for validating the U-Net-based Stable Diffusion architecture. This ensures the model can effectively predict and remove noise while generating high-quality, conditioned outputs.



Code:

import torch

import torchvision

from torchvision import transforms

import matplotlib.pyplot as plt

import torchvision.datasets as datasets

import torchvision.transforms as transforms

```
# Define transformations for CIFAR-10
```

```
transform = transforms.Compose([
transforms.Resize((32, 32)), # Ensure images are resized to 32x32
transforms.ToTensor(), # Convert images to PyTorch tensors
transforms.Normalize(mean=(0.5, 0.5, 0.5), std=(0.5, 0.5, 0.5)) # Normalize to [-1, 1]
])
```

Load CIFAR-10 dataset

```
train_dataset = datasets.CIFAR10(root='./data', train=True, transform=transform,
download=True)
```

```
train_loader = torch.utils.data.DataLoader(train dataset, batch size=64, shuffle=True,
num workers=4, pin memory=True)
# Denormalization function
def denormalize(img):
  img = (img * 0.5) + 0.5 # Reverse the normalization (assuming mean=0.5, std=0.5)
  return img
unique images, unique labels = next(iter(train loader))
unique images = unique images.permute(0, 2, 3, 1).numpy() # Permute to (batch, height,
width, channels)
unique images = denormalize(unique images) # Denormalize to [0, 1]
fig, axes = plt.subplots(4, 16, figsize=(16, 4), sharex=True, sharey=True) # Create a 4x16 grid
of subplots with a wider figure
for i in range(4): # Loop over rows
  for j in range(16): # Loop over columns
     index = i * 16 + j # Calculate the index in the batch
     axes[i, j].imshow(unique images[index]) # Show the image
     axes[i, j].axis('off') # Turn off axis labels and ticks
plt.tight layout()
plt.show()
%%capture
# Install the 'einops' library for easy manipulation of tensors
!pip install einops
# Install the 'lpips' library for computing perceptual similarity between images
```

```
!pip install lpips
# Import the PyTorch library for tensor operations.
import torch
# Import the neural network module from PyTorch.
import torch.nn as nn
# Import functional operations from PyTorch.
import torch.nn.functional as F
# Import the 'numpy' library for numerical operations.
import numpy as np
# Import the 'functools' module for higher-order functions.
import functools
# Import the Adam optimizer from PyTorch.
from torch.optim import Adam
# Import the DataLoader class from PyTorch for handling datasets.
from torch.utils.data import DataLoader
# Import data transformation functions from torchvision.
import torchvision.transforms as transforms
# Import the CIFAR10 dataset from torchvision.
from torchvision.datasets import CIFAR10
# Import 'tqdm' for creating progress bars during training.
import tqdm
```

```
# Import 'trange' and 'tqdm' specifically for notebook compatibility.
from tqdm.notebook import trange, tqdm
# Import the learning rate scheduler from PyTorch.
from torch.optim.lr_scheduler import MultiplicativeLR, LambdaLR
# Import the 'matplotlib.pyplot' library for plotting graphs.
import matplotlib.pyplot as plt
# Import the 'make grid' function from torchvision.utils for visualizing image grids.
from torchvision.utils import make grid
# Importing the rearrange function from the einops library
from einops import rearrange
# Importing the math module for mathematical operations
import math
# Forward diffusion for N steps in 1D.
def forward diffusion 1D(x0, noise strength fn, t0, nsteps, dt):
  Parameters:
  - x0: Initial sample value (scalar)
  - noise strength fn: Function of time, outputs scalar noise strength
  - t0: Initial time
  - nsteps: Number of diffusion steps
  - dt: Time step size
```

Returns:

- x: Trajectory of sample values over time

```
- t: Corresponding time points for the trajectory
  ,,,,,,
  # Initialize the trajectory array
  x = np.zeros(nsteps + 1)
  # Set the initial sample value
  x[0] = x0
  # Generate time points for the trajectory
  t = t0 + np.arange(nsteps + 1) * dt
  # Perform Euler-Maruyama time steps for diffusion simulation
  for i in range(nsteps):
     # Get the noise strength at the current time
     noise strength = noise strength fn(t[i])
     # Generate a random normal variable
     random normal = np.random.randn()
    # Update the trajectory using Euler-Maruyama method
    x[i+1] = x[i] + random normal * noise strength
  # Return the trajectory and corresponding time points
  return x, t
# Example noise strength function: always equal to 1
def noise strength constant(t):
  ,,,,,,
  Example noise strength function that returns a constant value (1).
```

```
Parameters:
  - t: Time parameter (unused in this example)
  Returns:
  - Constant noise strength (1)
  return 1
# Number of diffusion steps
nsteps = 100
# Initial time
t0 = 0
# Time step size
dt = 0.1
# Noise strength function
noise strength fn = noise strength constant
# Initial sample value
x0 = 0
# Number of tries for visualization
num_tries = 5
# Setting larger width and smaller height for the plot
plt.figure(figsize=(15, 3))
# Loop for multiple trials
```

```
for i in range(num tries):
  # Simulate forward diffusion
  x, t = forward diffusion <math>1D(x0, noise strength fn, t0, nsteps, dt)
  # Plot the trajectory
  plt.plot(t, x, label=f'Trial {i+1}') # Adding a label for each trial
# Labeling the plot
plt.xlabel('Time', fontsize=20)
plt.ylabel('Sample Value ($x$)', fontsize=20)
# Title of the plot
plt.title('Forward Diffusion Visualization', fontsize=20)
# Adding a legend to identify each trial
plt.legend()
# Show the plot
plt.show()
# Reverse diffusion for N steps in 1D.
def reverse diffusion 1D(x0, noise strength fn, score fn, T, nsteps, dt):
  ,,,,,,
  Parameters:
  - x0: Initial sample value (scalar)
  - noise strength fn: Function of time, outputs scalar noise strength
  - score fn: Score function
  - T: Final time
```

```
- nsteps: Number of diffusion steps
```

```
- dt: Time step size
```

np.sqrt(dt)

```
Returns:
- x: Trajectory of sample values over time
- t: Corresponding time points for the trajectory
# Initialize the trajectory array
x = np.zeros(nsteps + 1)
# Set the initial sample value
x[0] = x0
# Generate time points for the trajectory
t = np.arange(nsteps + 1) * dt
# Perform Euler-Maruyama time steps for reverse diffusion simulation
for i in range(nsteps):
  # Calculate noise strength at the current time
  noise strength = noise strength fn(T - t[i])
  # Calculate the score using the score function
  score = score fn(x[i], 0, noise strength, T - t[i])
  # Generate a random normal variable
  random normal = np.random.randn()
  # Update the trajectory using the reverse Euler-Maruyama method
```

x[i + 1] = x[i] + score * noise strength**2 * dt + noise strength * random normal *

```
# Return the trajectory and corresponding time points
  return x, t
# Example score function: always equal to 1
def score simple(x, x0, noise strength, t):
  ,,,,,,
  Parameters:
  - x: Current sample value (scalar)
  - x0: Initial sample value (scalar)
  - noise strength: Scalar noise strength at the current time
  - t: Current time
Returns:
  - score: Score calculated based on the provided formula
  ,,,,,,
  # Calculate the score using the provided formula
  score = -(x - x0) / ((noise strength**2) * t)
  # Return the calculated score
  return score
# Number of reverse diffusion steps
nsteps = 100
# Initial time for reverse diffusion
t0 = 0
# Time step size for reverse diffusion
dt = 0.1
```

```
# Function defining constant noise strength for reverse diffusion
noise strength fn = noise strength constant
# Example score function for reverse diffusion
score fn = score simple
# Initial sample value for reverse diffusion
x0 = 0
# Final time for reverse diffusion
T = 11
# Number of tries for visualization
num tries = 5
# Setting larger width and smaller height for the plot
plt.figure(figsize=(15, 3))
# Loop for multiple trials
for i in range(num_tries):
  # Draw from the noise distribution, which is diffusion for time T with noise strength 1
  x0 = np.random.normal(loc=0, scale=T)
  # Simulate reverse diffusion
  x, t = reverse diffusion <math>1D(x0, noise strength fn, score fn, T, nsteps, dt)
  # Plot the trajectory
  plt.plot(t, x, label=f'Trial {i+1}') # Adding a label for each trial
```

```
# Labeling the plot
plt.xlabel('Time', fontsize=20)
plt.ylabel('Sample Value ($x$)', fontsize=20)
# Title of the plot
plt.title('Reverse Diffusion Visualized', fontsize=20)
# Adding a legend to identify each trial
plt.legend()
# Show the plot
plt.show()
# Define a module for Gaussian random features used to encode time steps.
class GaussianFourierProjection(nn.Module):
  def init (self, embed dim, scale=30.):
     ,,,,,,
     Parameters:
     - embed dim: Dimensionality of the embedding (output dimension)
     - scale: Scaling factor for random weights (frequencies)
     super()._init_()
     # Randomly sample weights (frequencies) during initialization.
     # These weights (frequencies) are fixed during optimization and are not trainable.
     self.W = nn.Parameter(torch.randn(embed dim // 2) * scale, requires grad=False)
  def forward(self, x):
     Parameters:
     - x: Input tensor representing time steps
```

```
,,,,,,
     # Calculate the cosine and sine projections: Cosine(2 pi freq x), Sine(2 pi freq x)
     x \text{ proj} = x[:, \text{None}] * \text{self.W[None, :]} * 2 * \text{np.pi}
     # Concatenate the sine and cosine projections along the last dimension
     return torch.cat([torch.sin(x proj), torch.cos(x proj)], dim=-1)
# Define a module for a fully connected layer that reshapes outputs to feature maps.
class Dense(nn.Module):
  def _init_(self, input_dim, output_dim):
     ,,,,,,
     Parameters:
     - input_dim: Dimensionality of the input features
     - output dim: Dimensionality of the output features
     ,,,,,,
     super(). init ()
     # Define a fully connected layer
     self.dense = nn.Linear(input dim, output dim)
  def forward(self, x):
     Parameters:
     - x: Input tensor
     Returns:
     - Output tensor after passing through the fully connected layer
      and reshaping to a 4D tensor (feature map)
     ,,,,,,
```

Apply the fully connected layer and reshape the output to a 4D tensor

```
return self.dense(x)[..., None, None]
     # This broadcasts the 2D tensor to a 4D tensor, adding the same value across space.
# Define a time-dependent score-based model built upon the U-Net architecture.
class UNet(nn.Module):
  def init (self, marginal prob std, channels=[32, 64, 128, 256], embed dim=256):
     ,,,,,,
     Initialize a time-dependent score-based network.
     Parameters:
     - marginal prob std: A function that gives the standard deviation
      of the perturbation kernel p \{0t\}(x(t) \mid x(0)).
     - channels: The number of channels for feature maps of each resolution.
     - embed dim: The dimensionality of Gaussian random feature embeddings.
     ,,,,,,
     super(). init ()
     # Gaussian random feature embedding layer for time
     self.time embed = nn.Sequential(
       GaussianFourierProjection(embed dim=embed dim),
       nn.Linear(embed dim, embed dim)
     )
     # Encoding layers where the resolution decreases
     self.conv1 = nn.Conv2d(3, channels[0], kernel size=3, stride=1, padding=1, bias=False)
     self.dense1 = Dense(embed dim, channels[0])
     self.gnorm1 = nn.GroupNorm(4, num channels=channels[0])
    self.conv2 = nn.Conv2d(channels[0], channels[1], kernel size=3, stride=2, padding=1,
bias=False)
     self.dense2 = Dense(embed dim, channels[1])
     self.gnorm2 = nn.GroupNorm(32, num channels=channels[1])
```

```
self.conv3 = nn.Conv2d(channels[1], channels[2], kernel size=3, stride=2, padding=1,
bias=False)
    self.dense3 = Dense(embed dim, channels[2])
    self.gnorm3 = nn.GroupNorm(32, num channels=channels[2])
    self.conv4 = nn.Conv2d(channels[2], channels[3], kernel size=3, stride=2, padding=1,
bias=False)
    self.dense4 = Dense(embed dim, channels[3])
    self.gnorm4 = nn.GroupNorm(32, num channels=channels[3])
    # Decoding layers where the resolution increases
    self.tconv4 = nn.ConvTranspose2d(channels[3], channels[2], kernel size=3, stride=2,
padding=1, output padding=1, bias=False)
    self.dense5 = Dense(embed dim, channels[2])
    self.tgnorm4 = nn.GroupNorm(32, num channels=channels[2])
    self.tconv3 = nn.ConvTranspose2d(channels[2] * 2, channels[1], kernel size=3, stride=2,
padding=1, output padding=1, bias=False)
    self.dense6 = Dense(embed dim, channels[1])
    self.tgnorm3 = nn.GroupNorm(32, num channels=channels[1])
    self.tconv2 = nn.ConvTranspose2d(channels[1] * 2, channels[0], kernel size=3, stride=2,
padding=1, output padding=1, bias=False)
    self.dense7 = Dense(embed dim, channels[0])
    self.tgnorm2 = nn.GroupNorm(32, num channels=channels[0])
    self.tconv1 = nn.ConvTranspose2d(channels[0] * 2, 1, kernel size=3, stride=1,
padding=1)
    # The swish activation function
    self.act = lambda x: x * torch.sigmoid(x)
```

```
self.marginal prob std = marginal prob std
def forward(self, x, t, y=None):
 Forward pass of the UNet model.
 Parameters:
 - x: Input tensor.
 - t: Time tensor.
 - y: Optional target tensor.
 Returns:
 - h: Output tensor after passing through the UNet architecture.
 # Obtain the Gaussian random feature embedding for time t
 embed = self.act(self.time embed(t))
 # Encoding path
 h1 = self.conv1(x) + self.dense1(embed)
 h1 = self.act(self.gnorm1(h1))
 h2 = self.conv2(h1) + self.dense2(embed)
 h2 = self.act(self.gnorm2(h2))
 h3 = self.conv3(h2) + self.dense3(embed)
h3 = self.act(self.gnorm3(h3))
 h4 = self.conv4(h3) + self.dense4(embed)
 h4 = self.act(self.gnorm4(h4))
 # Decoding path
 h = self.tconv4(h4) + self.dense5(embed)
```

h = self.act(self.tgnorm4(h))

```
# Ensure matching dimensions before concatenating h and h3
   if h.size(-1) != h3.size(-1) or h.size(-2) != h3.size(-2):
      h3 = F.interpolate(h3, size=(h.size(-2), h.size(-1)), mode="nearest")
   h = self.tconv3(torch.cat([h, h3], dim=1)) + self.dense6(embed)
   h = self.act(self.tgnorm3(h))
   # Ensure matching dimensions before concatenating h and h2
   if h.size(-1) != h2.size(-1) or h.size(-2) != h2.size(-2):
      h2 = F.interpolate(h2, size=(h.size(-2), h.size(-1)), mode="nearest")
   h = self.tconv2(torch.cat([h, h2], dim=1)) + self.dense7(embed)
   h = self.act(self.tgnorm2(h))
   # Ensure matching dimensions before concatenating h and h1
   if h.size(-1) != h1.size(-1) or h.size(-2) != h1.size(-2):
      h1 = F.interpolate(h1, size=(h.size(-2), h.size(-1)), mode="nearest")
   h = self.tconv1(torch.cat([h, h1], dim=1))
   # Normalize the output
   h = h / self.marginal prob std(t)[:, None, None, None]
   return h
class UNet res(nn.Module):
  def init (self, marginal prob std, channels=[32, 64, 128, 256], embed dim=256):
    Initialize the alternate UNet model.
     Parameters:
```

```
- marginal prob std: A function that gives the standard deviation
     of the perturbation kernel p \{0t\}(x(t) \mid x(0)).
    - channels: The number of channels for feature maps of each resolution.
    - embed dim: The dimensionality of Gaussian random feature embeddings.
    super(). init ()
    # Gaussian random feature embedding layer for time
    self.time embed = nn.Sequential(
      GaussianFourierProjection(embed dim=embed dim),
      nn.Linear(embed dim, embed dim)
    )
    # Encoding layers where the resolution decreases
    self.conv1 = nn.Conv2d(3, channels[0], kernel size=3, stride=1, padding=1, bias=False)
# Update input channels
    self.dense1 = Dense(embed dim, channels[0])
    self.gnorm1 = nn.GroupNorm(4, num channels=channels[0])
    self.conv2 = nn.Conv2d(channels[0], channels[1], kernel size=3, stride=2, padding=1,
bias=False)
    self.dense2 = Dense(embed dim, channels[1])
    self.gnorm2 = nn.GroupNorm(32, num channels=channels[1])
    self.conv3 = nn.Conv2d(channels[1], channels[2], kernel size=3, stride=2, padding=1,
bias=False)
    self.dense3 = Dense(embed dim, channels[2])
    self.gnorm3 = nn.GroupNorm(32, num_channels=channels[2])
    self.conv4 = nn.Conv2d(channels[2], channels[3], kernel size=3, stride=2, padding=1,
bias=False)
    self.dense4 = Dense(embed dim, channels[3])
```

```
self.gnorm4 = nn.GroupNorm(32, num channels=channels[3])
    # Decoding layers where the resolution increases
    self.tconv4 = nn.ConvTranspose2d(channels[3], channels[2], kernel size=3, stride=2,
padding=1, output padding=1, bias=False)
    self.dense5 = Dense(embed dim, channels[2])
    self.tgnorm4 = nn.GroupNorm(32, num channels=channels[2])
    self.tconv3 = nn.ConvTranspose2d(channels[2], channels[1], kernel size=3, stride=2,
padding=1, output padding=1, bias=False)
    self.dense6 = Dense(embed dim, channels[1])
    self.tgnorm3 = nn.GroupNorm(32, num_channels=channels[1])
    self.tconv2 = nn.ConvTranspose2d(channels[1], channels[0], kernel size=3, stride=2,
padding=1, output padding=1, bias=False)
    self.dense7 = Dense(embed dim, channels[0])
    self.tgnorm2 = nn.GroupNorm(32, num channels=channels[0])
    self.tconv1 = nn.ConvTranspose2d(channels[0], 1, kernel size=3, stride=1, padding=1)
    # The swish activation function
    self.act = lambda x: x * torch.sigmoid(x)
    self.marginal prob std = marginal prob std
  def forward(self, x, t, y=None):
    ,,,,,,
    Parameters:
    - x: Input tensor
    - t: Time tensor
    - y: Target tensor (not used in this forward pass)
```

Returns:

```
- h: Output tensor after passing through the U-Net architecture
# Obtain the Gaussian random feature embedding for t
embed = self.act(self.time embed(t))
# Encoding path
h1 = self.conv1(x) + self.dense1(embed)
h1 = self.act(self.gnorm1(h1))
h2 = self.conv2(h1) + self.dense2(embed)
h2 = self.act(self.gnorm2(h2))
h3 = self.conv3(h2) + self.dense3(embed)
h3 = self.act(self.gnorm3(h3))
h4 = self.conv4(h3) + self.dense4(embed)
h4 = self.act(self.gnorm4(h4))
# Decoding path
h = self.tconv4(h4)
h += self.dense5(embed)
h = self.act(self.tgnorm4(h))
h = self.tconv3(h + h3)
h += self.dense6(embed)
h = self.act(self.tgnorm3(h))
h = self.tconv2(h + h2)
h += self.dense7(embed)
h = self.act(self.tgnorm2(h))
h = self.tconv1(h + h1)
# Normalize output
```

```
h = h / self.marginal_prob_std(t)[:, None, None, None]
    return h
# Using GPU
device = "cuda"
# Marginal Probability Standard Deviation Function
def marginal prob std(t, sigma):
  Compute the mean and standard deviation of p_{0}(x(t) | x(0)).
  Parameters:
  - t: A vector of time steps.
  - sigma: The $\sigma$ in our SDE.
  Returns:
  - The standard deviation.
  ,,,,,,
  # Convert time steps to a PyTorch tensor
  t = torch.tensor(t, device=device)
  #t = t.clone().detach().to(device)
  # Calculate and return the standard deviation based on the given formula
  return torch.sqrt((sigma**(2 * t) - 1.) / 2. / np.log(sigma))
# Using GPU
device = "cuda"
def diffusion coeff(t, sigma):
  Compute the diffusion coefficient of our SDE.
```

Parameters:

```
- t: A vector of time steps.
```

```
- sigma: The $\sigma$ in our SDE.
```

Returns:

- The vector of diffusion coefficients.

,,,,,

Calculate and return the diffusion coefficients based on the given formula return torch.tensor(sigma**t, device=device)

```
# Sigma Value
sigma = 25.0
```

```
# marginal probability standard
```

```
marginal prob std fn = functools.partial(marginal prob std, sigma=sigma)
```

diffusion coefficient

```
diffusion_coeff_fn = functools.partial(diffusion_coeff, sigma=sigma)
def loss_fn(model, x, marginal_prob_std, eps=1e-5):
```

,,,,,,

The loss function for training score-based generative models.

Parameters:

- model: A PyTorch model instance that represents a time-dependent score-based model.
- x: A mini-batch of training data.
- marginal prob std: A function that gives the standard deviation of the perturbation kernel.
- eps: A tolerance value for numerical stability.

,,,,,

```
# Sample time uniformly in the range (eps, 1-eps)
```

```
random t = \text{torch.rand}(x.\text{shape}[0], \text{device}=x.\text{device}) * (1. - 2 * \text{eps}) + \text{eps}
```

```
# Find the noise std at the sampled time t
  std = marginal prob std(random t)
  # Generate normally distributed noise
  z = torch.randn like(x)
  # Perturb the input data with the generated noise
  perturbed_x = x + z * std[:, None, None, None]
  # Get the score from the model using the perturbed data and time
  score = model(perturbed x, random t)
  # Ensure score and noise have matching dimensions
  if score.size() != z.size():
    z = F.interpolate(z, size=score.shape[2:], mode='bilinear', align corners=False)
  # Calculate the loss based on the score and noise
  loss = torch.mean(torch.sum((score * std[:, None, None, None] + z)**2, dim=(1, 2, 3)))
  return loss
def Euler Maruyama sampler(score model,
                marginal prob std,
                diffusion coeff,
                batch size=64,
                x \text{ shape}=(3, 32, 32),
                num steps=1000,
                device='cuda',
                eps=1e-3,
                y=None):
```

Applied Machine Learning ****** Generate samples using Euler-Maruyama sampler with corrected sqrt() usage. ****** t = torch.ones(batch_size, device=device) init x = torch.randn(batch size, *x shape, device=device) * marginal prob std(t)[:, None, None, None] time steps = torch.linspace(1., eps, num steps, device=device) step size = time steps[0] - time steps[1]x = init xwith torch.no grad(): for time step in time steps: batch time step = torch.ones(batch size, device=device) * time step g = diffusion coeff(batch time step) mean $x = x + (g^{**}2)[:, None, None, None] * score model(x, batch time step, y=y) *$ step size noise = torch.randn like(x) x = mean x + torch.sqrt(torch.tensor(step size, device=device)) * g[:, None, None,None] * noise return x # Define the score-based model and move it to the specified device score model = torch.nn.DataParallel(UNet(marginal prob std=marginal prob std fn)) score model = score model.to(device)

```
# Number of training epochs
n epochs = 150
# Size of a mini-batch
batch size = 256
# Learning rate
```

```
# Load the CIFAR10 dataset and create a data loader
dataset = CIFAR10('.', train=True, transform=transforms.Compose([transforms.Resize((32,
32)), transforms.ToTensor(), transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5))]),
download=True)
data loader = DataLoader(dataset, batch size=batch size, shuffle=True, num workers=2)
# Define the Adam optimizer for training the model
optimizer = Adam(score model.parameters(), lr=lr)
# Progress bar for epochs
tqdm epoch = trange(n epochs)
for epoch in tqdm epoch:
  avg loss = 0.
  num items = 0
  # Iterate through mini-batches in the data loader
  for x, y in tqdm(data loader):
    x = x.to(device)
    # Calculate the loss and perform backpropagation
    loss = loss fn(score model, x, marginal prob std fn)
    optimizer.zero grad()
    loss.backward()
    optimizer.step()
    avg loss += loss.item() * x.shape[0]
    num items += x.shape[0]
  # Print the averaged training loss for the current epoch
  tqdm epoch.set description('Average Loss: {:5f}'.format(avg loss / num items))
  # Save the model checkpoint after each epoch of training
  torch.save(score model.state dict(), 'ckpt.pth')
# Load the pre-trained checkpoint from disk
```

```
device = 'cuda'
# Load the pre-trained model checkpoint
ckpt = torch.load('ckpt.pth', map location=device, weights only=True)
                                                                                     Set
weights_only=True
score model.load state dict(ckpt)
# Set sample batch size and number of steps
sample batch size = 64
num steps = 1000
# Choose the Euler-Maruyama sampler
sampler = Euler Maruyama sampler
# Generate samples using the specified sampler
samples = sampler(
  score model,
  marginal_prob_std_fn,
  diffusion coeff fn,
  sample batch size,
  num_steps=num_steps,
  device=device,
  y=None
)
# Clip samples to be in the range [0, 1]
samples = samples.clamp(0.0, 1.0)
# Visualize the generated samples
%matplotlib inline
```

import matplotlib.pyplot as plt

```
sample grid = make grid(samples, nrow=int(np.sqrt(sample batch size)))
# Plot the sample grid
plt.figure(figsize=(6, 6))
plt.axis('off')
plt.imshow(sample grid.permute(1, 2, 0).cpu(), vmin=0., vmax=1.)
plt.show()
# Initialize the alternate U-Net model for training.
score model = torch.nn.DataParallel(UNet res(marginal prob std=marginal prob std fn))
score model = score model.to(device)
# Set the number of training epochs, mini-batch size, and learning rate.
n epochs = 150
batch size = 256
lr = 1e-4
# Load the CIFAR10 dataset for training.
dataset = CIFAR10('.', train=True, transform=transforms.Compose([transforms.Resize((32,
32)), transforms.ToTensor(), transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5))]),
download=True)
data loader = DataLoader(dataset, batch size=batch size, shuffle=True, num workers=4)
# Initialize the Adam optimizer with the specified learning rate.
optimizer = Adam(score model.parameters(), lr=lr)
# Learning rate scheduler to adjust the learning rate during training.
scheduler = LambdaLR(optimizer, lr lambda=lambda epoch: max(0.2, 0.98 ** epoch))
# Training loop over epochs.
tqdm epoch = trange(n epochs)
for epoch in tqdm epoch:
```

```
avg_loss = 0.
  num items = 0
  # Iterate over mini-batches in the training data loader.
  for x, y in data loader:
    \#x = x.to(device)
    x, y = x.to(device), y.to(device)
     # Compute the loss for the current mini-batch.
     loss = loss_fn(score_model, x, marginal_prob_std_fn)
    # Zero the gradients, backpropagate, and update the model parameters.
     optimizer.zero grad()
     loss.backward()
     optimizer.step()
     # Accumulate the total loss and the number of processed items.
     avg loss += loss.item() * x.shape[0]
    num items += x.shape[0]
  # Adjust the learning rate using the scheduler.
  scheduler.step()
  lr current = scheduler.get last lr()[0]
  # Print the average loss and learning rate for the current epoch.
  print('{} Average Loss: {:5f} lr {:.1e}'.format(epoch, avg loss / num items, lr current))
  tqdm epoch.set description('Average Loss: {:5f}'.format(avg loss / num items))
  # Save the model checkpoint after each epoch of training.
  torch.save(score model.state dict(), 'ckpt res.pth')
# Load the pre-trained checkpoint from disk.
device = 'cuda'
# Load the pre-trained model checkpoint
```

```
ckpt = torch.load('ckpt res.pth', map location=device)
score model.load state dict(ckpt)
# Set sample batch size and number of steps
sample_batch_size = 64
num steps = 1000
# Choose the Euler-Maruyama sampler
sampler = Euler_Maruyama_sampler
# Generate samples using the specified sampler
samples = sampler(score model,
          marginal prob std fn,
          diffusion coeff fn,
          sample batch size,
          num steps=num steps,
          device=device,
          y=None)
# Clip samples to be in the range [0, 1]
samples = samples.clamp(0.0, 1.0)
# Visualize the generated samples
%matplotlib inline
import matplotlib.pyplot as plt
sample grid = make grid(samples, nrow=int(np.sqrt(sample batch size)))
# Plot the sample grid
plt.figure(figsize=(6, 6))
plt.axis('off')
```

```
plt.imshow(sample grid.permute(1, 2, 0).cpu(), vmin=0., vmax=1.)
plt.show()
class CrossAttention(nn.Module):
  def init (self, embed dim, hidden dim, context dim=None, num heads=1):
     ,,,,,,
     Initialize the CrossAttention module.
     Parameters:
     - embed dim: The dimensionality of the output embeddings.
     - hidden dim: The dimensionality of the hidden representations.
    - context dim: The dimensionality of the context representations (if not self attention).
     - num heads: Number of attention heads (currently supports 1 head).
    Note: For simplicity reasons, the implementation assumes 1-head attention.
     Feel free to implement multi-head attention using fancy tensor manipulations.
     ,,,,,,
     super(CrossAttention, self). init ()
     self.hidden dim = hidden dim
     self.context dim = context dim
     self.embed dim = embed dim
     # Linear layer for query projection
     self.query = nn.Linear(hidden dim, embed dim, bias=False)
     # Check if self-attention or cross-attention
     if context dim is None:
       self.self attn = True
       self.key = nn.Linear(hidden dim, embed dim, bias=False)
```

```
self.value = nn.Linear(hidden dim, hidden dim, bias=False)
  else:
    self.self attn = False
    self.key = nn.Linear(context dim, embed dim, bias=False)
    self.value = nn.Linear(context dim, hidden dim, bias=False)
def forward(self, tokens, context=None):
  Forward pass of the CrossAttention module.
  Parameters:
  - tokens: Input tokens with shape [batch, sequence_len, hidden_dim].
  - context: Context information with shape [batch, context seq len, context dim].
         If self attn is True, context is ignored.
  Returns:
  - ctx vecs: Context vectors after attention with shape [batch, sequence len, embed dim].
  ******
  if self.self attn:
    # Self-attention case
    Q = self.query(tokens)
    K = self.key(tokens)
    V = self.value(tokens)
  else:
    # Cross-attention case
    Q = self.query(tokens)
    K = self.key(context)
    V = self.value(context)
```

```
# Compute score matrices, attention matrices, and context vectors
    scoremats = torch.einsum("BTH,BSH->BTS", Q, K) # Inner product of Q and K, a tensor
    attnmats = F.softmax(scoremats / math.sqrt(self.embed_dim), dim=-1) # Softmax of
scoremats
    ctx_vecs = torch.einsum("BTS,BSH->BTH", attnmats, V) # Weighted average value
vectors by attnmats
    return ctx vecs
class TransformerBlock(nn.Module):
  """The transformer block that combines self-attn, cross-attn, and feed forward neural net"""
  def _init_(self, hidden_dim, context_dim):
    Initialize the TransformerBlock.
    Parameters:
    - hidden dim: The dimensionality of the hidden state.
    - context dim: The dimensionality of the context tensor.
    Note: For simplicity, the self-attn and cross-attn use the same hidden dim.
    ** ** **
    super(TransformerBlock, self). init ()
    # Self-attention module
    self.attn self = CrossAttention(hidden dim, hidden dim)
    # Cross-attention module
    self.attn cross = CrossAttention(hidden dim, hidden dim, context dim)
    # Layer normalization modules
    self.norm1 = nn.LayerNorm(hidden dim)
```

```
self.norm2 = nn.LayerNorm(hidden dim)
  self.norm3 = nn.LayerNorm(hidden dim)
  # Implement a 2-layer MLP with K * hidden dim hidden units, and nn.GELU nonlinearity
  self.ffn = nn.Sequential(
    nn.Linear(hidden dim, 3 * hidden dim),
    nn.GELU(),
    nn.Linear(3 * hidden dim, hidden dim)
  )
def forward(self, x, context=None):
  Forward pass of the TransformerBlock.
  Parameters:
  - x: Input tensor with shape [batch, sequence len, hidden dim].
  - context: Context tensor with shape [batch, context seq len, context dim].
  Returns:
  - x: Output tensor after passing through the TransformerBlock.
  # Apply self-attention with layer normalization and residual connection
  x = self.attn self(self.norm1(x)) + x
  # Apply cross-attention with layer normalization and residual connection
  x = self.attn\_cross(self.norm2(x), context=context) + x
  # Apply feed forward neural network with layer normalization and residual connection
  x = self.ffn(self.norm3(x)) + x
```

```
return x
class SpatialTransformer(nn.Module):
  def init (self, hidden dim, context dim):
     ,,,,,,
    Initialize the SpatialTransformer.
    Parameters:
    - hidden_dim: The dimensionality of the hidden state.
    - context dim: The dimensionality of the context tensor.
     ,,,,,,
    super(SpatialTransformer, self). init ()
     # TransformerBlock for spatial transformation
    self.transformer = TransformerBlock(hidden dim, context dim)
  def forward(self, x, context=None):
    Forward pass of the SpatialTransformer.
     Parameters:
    - x: Input tensor with shape [batch, channels, height, width].
    - context: Context tensor with shape [batch, context seq len, context dim].
     Returns:
    - x: Output tensor after applying spatial transformation.
    b, c, h, w = x.shape
    x in = x
```

```
# Combine the spatial dimensions and move the channel dimension to the end
    x = rearrange(x, "b c h w -> b (h w) c")
    # Apply the sequence transformer
    x = self.transformer(x, context)
    # Reverse the process
    x = rearrange(x, 'b (h w) c \rightarrow b c h w', h=h, w=w)
    # Residue connection
    return x + x in
class UNet Tranformer(nn.Module):
  """A time-dependent score-based model built upon U-Net architecture."""
  def init (self, marginal prob std, channels=[32, 64, 128, 256], embed dim=256,
          text dim=256, nClass=10):
    ,,,,,,
    Initialize a time-dependent score-based network.
    Parameters:
    - marginal prob std: A function that gives the standard deviation
     of the perturbation kernel p_{0}(x(t) | x(0)).
    - channels: The number of channels for feature maps of each resolution.
    - embed dim: The dimensionality of Gaussian random feature embeddings of time.
    - text dim: The embedding dimension of text/digits.
    - nClass: Number of classes to model.
    super(). init ()
    # Gaussian random feature embedding layer for time
    self.time embed = nn.Sequential(
```

```
GaussianFourierProjection(embed dim=embed dim),
      nn.Linear(embed dim, embed dim)
    )
    # Encoding layers where the resolution decreases
    self.conv1 = nn.Conv2d(3, channels[0], kernel size=3, stride=1, padding=1, bias=False)
# Updated to 3 channels
    self.dense1 = Dense(embed dim, channels[0])
    self.gnorm1 = nn.GroupNorm(4, num channels=channels[0])
    self.conv2 = nn.Conv2d(channels[0], channels[1], kernel size=3, stride=2, padding=1,
bias=False)
    self.dense2 = Dense(embed_dim, channels[1])
    self.gnorm2 = nn.GroupNorm(32, num channels=channels[1])
    self.conv3 = nn.Conv2d(channels[1], channels[2], kernel size=3, stride=2, padding=1,
bias=False)
    self.dense3 = Dense(embed dim, channels[2])
    self.gnorm3 = nn.GroupNorm(32, num channels=channels[2])
    self.attn3 = SpatialTransformer(channels[2], text_dim)
    self.conv4 = nn.Conv2d(channels[2], channels[3], kernel size=3, stride=2, padding=1,
bias=False)
    self.dense4 = Dense(embed dim, channels[3])
    self.gnorm4 = nn.GroupNorm(32, num channels=channels[3])
    self.attn4 = SpatialTransformer(channels[3], text_dim)
    # Decoding layers where the resolution increases
    self.tconv4 = nn.ConvTranspose2d(channels[3], channels[2], kernel size=3, stride=2,
padding=1, output padding=1, bias=False)
    self.dense5 = Dense(embed dim, channels[2])
    self.tgnorm4 = nn.GroupNorm(32, num channels=channels[2])
```

```
self.tconv3 = nn.ConvTranspose2d(channels[2], channels[1], kernel size=3, stride=2,
padding=1, output padding=1, bias=False)
    self.dense6 = Dense(embed dim, channels[1])
    self.tgnorm3 = nn.GroupNorm(32, num channels=channels[1])
    self.tconv2 = nn.ConvTranspose2d(channels[1], channels[0], kernel size=3, stride=2,
padding=1, output padding=1, bias=False)
    self.dense7 = Dense(embed dim, channels[0])
    self.tgnorm2 = nn.GroupNorm(32, num channels=channels[0])
    self.tconv1 = nn.ConvTranspose2d(channels[0], 3, kernel size=3, stride=1, padding=1) #
Fixed to output 3 channels
    # The swish activation function
    self.act = nn.SiLU()
    self.marginal prob std = marginal prob std
    self.cond embed = nn.Embedding(nClass, text dim)
  def forward(self, x, t, y=None):
    Forward pass of the UNet Transformer model.
    Parameters:
    - x: Input tensor.
    - t: Time tensor.
    - y: Target tensor.
    Returns:
    - h: Output tensor after passing through the UNet Transformer architecture.
```

```
,,,,,,
```

```
# Obtain the Gaussian random feature embedding for t
embed = self.act(self.time embed(t))
y embed = self.cond embed(y).unsqueeze(1)
# Encoding path
h1 = self.conv1(x) + self.dense1(embed)
h1 = self.act(self.gnorm1(h1))
h2 = self.conv2(h1) + self.dense2(embed)
h2 = self.act(self.gnorm2(h2))
h3 = self.conv3(h2) + self.dense3(embed)
h3 = self.act(self.gnorm3(h3))
h3 = self.attn3(h3, y embed)
h4 = self.conv4(h3) + self.dense4(embed)
h4 = self.act(self.gnorm4(h4))
h4 = self.attn4(h4, y embed)
# Decoding path
h = self.tconv4(h4) + self.dense5(embed)
h = self.act(self.tgnorm4(h))
h = self.tconv3(h + h3) + self.dense6(embed)
h = self.act(self.tgnorm3(h))
h = self.tconv2(h + h2) + self.dense7(embed)
h = self.act(self.tgnorm2(h))
h = self.tconv1(h + h1)
# Normalize output
h = h / self.marginal prob std(t)[:, None, None, None]
return h
```

```
def loss_fn_cond(model, x, y, marginal_prob_std, eps=1e-5):
```

The loss function for training score-based generative models with conditional information.

Parameters:

- model: A PyTorch model instance that represents a time-dependent score-based model.
- x: A mini-batch of training data.
- y: Conditional information (target tensor).
- marginal_prob_std: A function that gives the standard deviation of the perturbation kernel.
- eps: A tolerance value for numerical stability.

Returns:

```
- loss: The calculated loss.

# Sample time uniformly in the range [eps, 1-eps]

random_t = torch.rand(x.shape[0], device=x.device) * (1. - eps) + eps

# Generate random noise with the same shape as the input

z = torch.randn_like(x)

# Compute the standard deviation of the perturbation kernel at the sampled time

std = marginal_prob_std(random_t)

# Perturb the input data with the generated noise and scaled by the standard deviation

perturbed_x = x + z * std[:, None, None, None]

# Get the model's score for the perturbed input, considering conditional information

score = model(perturbed_x, random_t, y=y)

# Calculate the loss using the score and perturbation

loss = torch.mean(torch.sum((score * std[:, None, None, None] + z)**2, dim=(1, 2, 3)))

return loss
```

Specify whether to continue training or initialize a new model

```
continue training = False # Either True or False
```

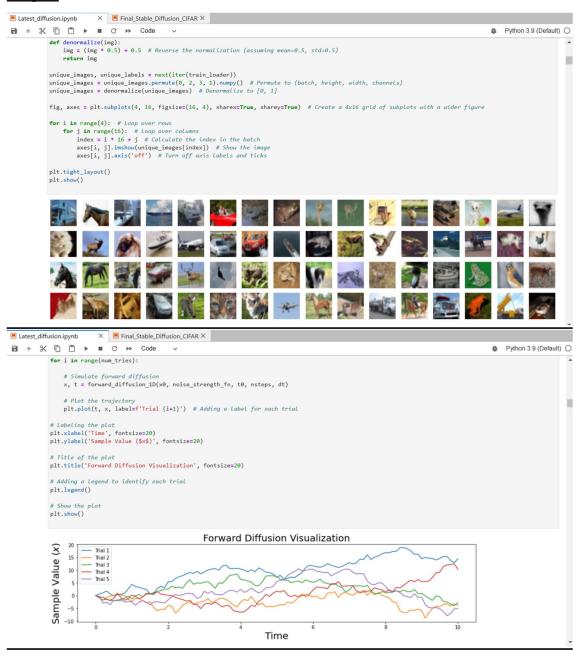
```
if not continue training:
  # Initialize a new UNet with Transformer model
  score model
                                                                                        =
torch.nn.DataParallel(UNet Tranformer(marginal prob std=marginal prob std fn))
  score model = score model.to(device)
# Set training hyperparameters
n epochs = 200 #{'type':'integer'}
batch size = 256 #{'type':'integer'}
lr = 1e-4
             #{'type':'number'}
# Load the CIFAR10 dataset and create a data loader
dataset = CIFAR10('.', train=True, transform=transforms.Compose([transforms.Resize((32,
32)), transforms.ToTensor(), transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5))]),
download=True)
data loader = DataLoader(dataset, batch size=batch size, shuffle=True, num workers=4)
# Define the optimizer and learning rate scheduler
optimizer = Adam(score model.parameters(), lr=lr)
scheduler = LambdaLR(optimizer, lr lambda=lambda epoch: max(0.2, 0.98 ** epoch))
# Use tqdm to display a progress bar over epochs
tqdm epoch = trange(n epochs)
for epoch in tqdm epoch:
  avg loss = 0.
```

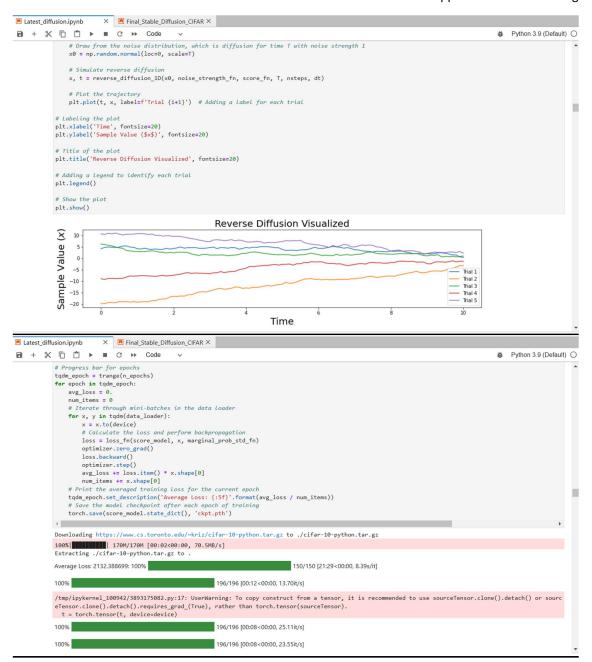
num items = 0

```
# Iterate over batches in the data loader
  for x, y in tqdm(data loader):
    \#x = x.to(device)
    x, y = x.to(device), y.to(device)
    # Compute the loss using the conditional score-based model
    loss = loss fn cond(score model, x, y, marginal prob std fn)
     optimizer.zero grad()
     loss.backward()
    optimizer.step()
    avg loss += loss.item() * x.shape[0]
     num items += x.shape[0]
  # Adjust learning rate using the scheduler
  scheduler.step()
  lr current = scheduler.get last lr()[0]
  # Print epoch information including average loss and current learning rate
  print('{} Average Loss: {:5f} lr {:.1e}'.format(epoch, avg loss / num items, lr current))
  tqdm epoch.set description('Average Loss: {:5f}'.format(avg loss / num items))
  # Save the model checkpoint after each epoch of training
  torch.save(score model.state dict(), 'ckpt transformer.pth')
# Load model and generate samples
score model
torch.nn.DataParallel(UNet Tranformer(marginal prob std=marginal prob std fn))
ckpt = torch.load('ckpt_transformer.pth', map_location=device)
score model.load state dict(ckpt)
score model.eval()
target class = 3
```

```
samples = Euler_Maruyama_sampler(
  score model,
  marginal_prob_std_fn,
  diffusion_coeff_fn,
  batch size=64,
  x \text{ shape}=(3, 32, 32),
  num steps=250,
  device=device,
  y=target_class * torch.ones(64, dtype=torch.long, device=device)
)
# Visualize samples
samples = samples.clamp(0.0, 1.0)
sample grid = make grid(samples, nrow=8)
plt.figure(figsize=(8, 8))
plt.axis('off')
plt.imshow(sample grid.permute(1, 2, 0).cpu(), vmin=0., vmax=1.)
plt.title(f"Generated Samples for Class {target class}")
plt.show()
```

Output:





Applied Machine Learning

