

Homework 3: Diffusion Models

CSC 8851 – Deep Learning - Fall 2025

Learning Objectives

- Implement a linear noise schedule and visualize the forward diffusion process.
- Use `diffusers` components: `UNet2DModel`, `DDPMScheduler`, and `DDIMScheduler`.
- Train a class-conditional denoiser that predicts x_0 and implement classifier-free guidance (CFG).
- Sample with DDPM (full steps) and DDIM (short trajectory) using CFG; compare speed/quality.

Assignment Tasks (100 pts)

Part 1: Linear Noise Schedule and Forward Noising (10 pts)

Let $T = 1000$. Define per-step quantities

$$\beta_t \in (0, 1), \quad \alpha_t = 1 - \beta_t, \quad \bar{\alpha}_t = \prod_{i=0}^t \alpha_i, \quad t = 0, \dots, T-1,$$

with a **linear** progression $\beta_t \in [10^{-4}, 2 \cdot 10^{-2}]$. The forward (noising) process is

$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t)\mathbf{I}) \iff \mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim \mathcal{N}(0, \mathbf{I}).$$

- (5 pts) Compute and plot $\{\beta_t\}$, $\{\alpha_t\}$, and $\{\bar{\alpha}_t\}$ vs. t (three plots). See Figure 1a.
- (5 pts) For one MNIST image, visualize \mathbf{x}_t at `steps=[0, 50, 100, 200, 250, 300, 400, 500, 600, 700, 800, 999]`. See Figure 1b. **Note:** Scale images to $[-1, 1]$.

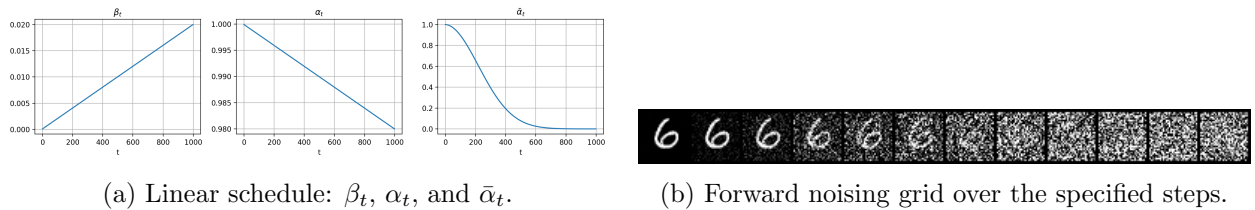


Figure 1: Part 1 diagnostics.

Note (not required): A *cosine* schedule designs $\bar{\alpha}_t$ via a smooth target curve that preserves more signal early and can stabilize training; we only implement **linear** here.

Part 2: Model and Schedulers (PyTorch Diffusers) (20 pts)

- `UNet2DModel`: convolutional U-Net that accepts an input tensor and a discrete timestep t . In our setup it predicts $\hat{\mathbf{x}}_0$ (`prediction_type="sample"`).

UNet2DModel configuration (Do not change the architecture).

```
sample_size = 32,  in_channels = 1 + 10,  out_channels = 1

layers_per_block = 2,  block_out_channels = (32, 64, 128),
down_block_types = ("DownBlock2D", "DownBlock2D", "DownBlock2D")
up_block_types = ("UpBlock2D", "UpBlock2D", "UpBlock2D").
```

UNet2DModel architecture. Input $\mathbf{Z} \in \mathbb{R}^{B \times 11 \times 32 \times 32}$ flows through:

1. **Time embedding:** sinusoidal \rightarrow MLP \rightarrow injected into ResNet blocks.
 2. **Encoder (Down path):** three stages with two ResNet blocks each; channels $11 \rightarrow 32 \rightarrow 64 \rightarrow 128$; spatial downsample $32 \rightarrow 16 \rightarrow 8 \rightarrow 4$. Skip connections saved.
 3. **Mid block:** ResNet(s) at $(B, 128, 4, 4)$.
 4. **Decoder (Up path):** three stages with skip concatenations; channels $128 \rightarrow 64 \rightarrow 32$; spatial upsample $4 \rightarrow 8 \rightarrow 16 \rightarrow 32$.
 5. **Output head:** 3×3 conv $\rightarrow (B, 1, 32, 32)$ giving $\hat{\mathbf{x}}_0$ (no final activation).
- **DDPMScheduler:**
 - Training (forward noising): $\mathbf{X}_t = \text{ddpm.add_noise}(\mathbf{X}_0, \text{eps}, t)$ implements $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \varepsilon$.
 - Sampling (reverse): `ddpm.set_timesteps(N)` then iterate $t \in \text{ddpm.timesteps}$ and call `ddpm.step(model_output= $\hat{\mathbf{x}}_0$, timestep= t , sample= \mathbf{X})` to obtain the next sample.
 - With `prediction_type="sample"`, `model_output` must be $\hat{\mathbf{x}}_0$ (your network output).
 - **DDIMScheduler:**
 - Same API as DDPM but supports a shortened, non-Markovian trajectory; set `ddim.set_timesteps(K)` with $K \ll T$.
 - The call `ddim.step(model_output= $\hat{\mathbf{x}}_0$, timestep= t , sample= \mathbf{X} , eta=0.0)` yields the deterministic DDIM update.

DDPMScheduler and DDIMScheduler configuration

```
num_train_timesteps = T,  beta_schedule = "linear",  prediction_type = "sample"
```

- **Class conditioning (one-hot planes).** Given labels $y \in \{0, \dots, 9\}^B$, build one-hot class maps $\mathbf{C} \in \mathbb{R}^{B \times 10 \times H \times W}$ and concatenate with the (noised) image $\mathbf{X}_t \in \mathbb{R}^{B \times 1 \times H \times W}$ to form the model input:

$$\mathbf{Z}_t = [\mathbf{X}_t; \mathbf{C}] \in \mathbb{R}^{B \times 11 \times H \times W}, \quad H = W = 32.$$

Efficient construction: `F.one_hot(y, 10).float().view(B, 10, 1, 1).expand(B, 10, H, W)` (no per-pixel loops).

`make_model_input` (**training-time CFG dropout**). We randomly zero all class channels (dropout) for some samples to train the model to also handle *unconditional* inputs:

`make_model_input`($\mathbf{X}_t, y, p_{\text{uncond}}$) = $[\mathbf{X}_t; \mathbf{C} \odot \mathbf{M}]$, $\mathbf{M} \in \{0, 1\}^{B \times 1 \times 1 \times 1}$, $\Pr[M=0] = p_{\text{uncond}}$.

```
def make_model_input(x, y, p_uncond=0.1):
    B, _, H, W = x.shape
    C = F.one_hot(y, 10).float().view(B, 10, 1, 1).expand(B, 10, H, W)
    m = (torch.rand(B, device=x.device) < p_uncond).float().view(B, 1, 1, 1)
    C = C * (1.0 - m) # zero all class planes for some samples
    return torch.cat([x, C.to(x.dtype)], dim=1) # (B, 11, H, W)
```

How to use it.

- **Training:** always feed `make_model_input`($\mathbf{X}_t, y, p_{\text{uncond}}$) into `UNet2DModel`, where \mathbf{X}_t are noised images generated by `DDPMScheduler.add_noise`. The model predicts $\hat{\mathbf{x}}_0$; optimize $\text{MSE}(\hat{\mathbf{x}}_0, \mathbf{x}_0)$.
- **Sampling with CFG (Part 5):** build two inputs at each step: *conditional* $[\mathbf{X}_t; \mathbf{C}]$ and *unconditional* $[\mathbf{X}_t; \mathbf{0}]$, run the model on both, and combine

$$\hat{\mathbf{x}}_0^{\text{cfg}} = \hat{\mathbf{x}}_0^{\text{cond}} + s(\hat{\mathbf{x}}_0^{\text{cond}} - \hat{\mathbf{x}}_0^{\text{uncond}}), \quad s \geq 0.$$

Grading for Part 2 (20 pts).

- (10 pts) Correct instantiation of `UNet2DModel`, `DDPMScheduler`, and `DDIMScheduler` with the specified configuration; Evaluate a dummy forward: `model(Z,t).sample -> (B,1,32,32)` and verify shape.
- (10 pts) Implement `make_model_input` (correct shapes and dropout behavior).

Part 3: Training (50 epochs) and Curve (20 pts)

Train the UNet to predict \mathbf{x}_0 :

$$\mathbf{x}_t = \sqrt{\alpha_t} \mathbf{x}_0 + \sqrt{1 - \alpha_t} \varepsilon, \quad \mathcal{L} = \mathbb{E}[\|\hat{\mathbf{x}}_0(\mathbf{x}_t, y, t) - \mathbf{x}_0\|_2^2].$$

One-epoch training pseudocode (\mathbf{x}_0 prediction).

```
# Assumes: model (UNet2DModel), ddpm (DDPMScheduler), train_loader, optimizer 'opt'
model.train()
running, total, count = None, 0.0, 0
for X0, y in train_loader: # X0 in [-1,1], shape (B,1,32,32)
    X0 = X0.to(dev); y = y.to(dev).long()
    B = X0.size(0)

    # Sample t and construct forward noising (DDPM)
    t = torch.randint(0, ddpm.config.num_train_timesteps, (B,)),
        device=dev, dtype=torch.long)
```

```

eps = torch.randn_like(X0)
Xt = ddpm.add_noise(X0, eps, t)
# where  $x_t = \sqrt{\text{bar\_alpha\_t}} x_0 + \sqrt{1-\text{bar\_alpha\_t}} \text{eps}$ 

# Build conditional/unconditional-batch input with CFG dropout
Zt = make_model_input(Xt, y, p_uncond=0.1) # (B,11,32,32)

# Predict  $x_0$  and optimize  $\text{MSE}(x_0_{\text{hat}}, x_0)$ 
x0_hat = model(Zt, t).sample
loss = F.mse_loss(x0_hat, X0)

opt.zero_grad(set_to_none=True)
loss.backward()
opt.step()

# (Optional) track loss
total += float(loss.item()) * B; count += B
running = loss.item() if running is None else 0.98*running + 0.02*loss.item()

avg_loss = total / max(count, 1)
print(f"avg_epoch_loss={avg_loss:.4f}, running={running:.4f}")

```

- (15 pts) Implement loop: sample t , form \mathbf{x}_t via `ddpm.add_noise`, build inputs with `make_model_input`, predict $\hat{\mathbf{x}}_0$, optimize MSE.
- (5 pts) Plot the training loss. See Figure 2.

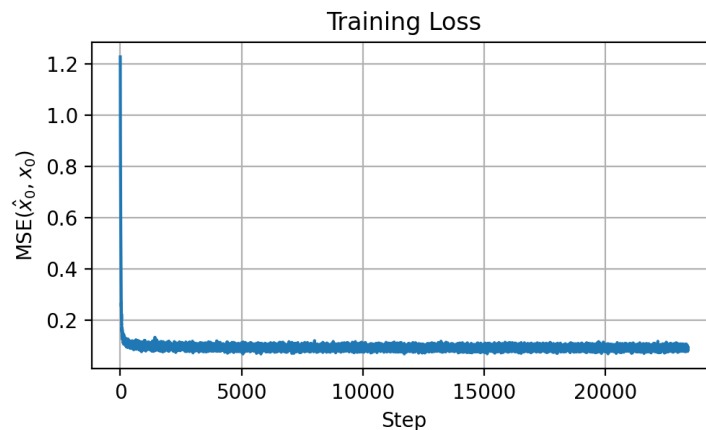


Figure 2: Training loss curve (MSE).

Part 4: Visualizing \hat{x}_0 Across Noise (20 pts)

Fix one (\mathbf{x}_0, y) . For the timesteps $[0, 50, 100, 200, 250, 300, 400, 500, 600, 700, 800, 999]$, form \mathbf{x}_t using the forward process and visualize the model's prediction $\hat{\mathbf{x}}_0(\mathbf{x}_t, \cdot, t)$ in two

settings:

- (10 pts) **Conditional** Use the *conditional* input (true label; no dropout): set $p_{\text{uncond}}=0$ inside your visualization helper so the class maps are active. See Figure: 3a.
- (10 pts) **Unconditional** Use the *unconditional* input by concatenating zero class maps (i.e., $[\mathbf{x}_t; \mathbf{0}]$). See Figure: 3b.



(a) Conditional \hat{x}_0 across timesteps (top: $t=0$; rightmost: $t=999$).



(b) Unconditional \hat{x}_0 across the same timesteps (zero class maps).

Figure 3: Part 5: \hat{x}_0 predictions across noise levels (conditional vs. unconditional).

Part 5: **Sampling — DDPM and DDIM with CFG** (30 pts)

At each step, form cond/uncond inputs, get $\hat{\mathbf{x}}_0^{\text{cond}}$, $\hat{\mathbf{x}}_0^{\text{uncond}}$, then $\hat{\mathbf{x}}_0^{\text{cfg}}$ with scale s .

- **5.1 DDPM Sampling** (15 pts). Use `DDPMScheduler` (`prediction_type="sample"`) and its reverse-time indices to iterate and update `X <- ddpm.step(...).prev_sample`. Generate a 10×8 class grid. See Figure 4a.
- **5.2 DDIM Sampling** (15 pts). DDIM uses a shortened, often deterministic ($\eta=0$) trajectory and works with a DDPM-trained model. Use 50 steps, $\eta=0$, and the same CFG combination; generate the same class grid and compare speed/quality vs. DDPM. See Figure 4b.

Submission Instructions

1. Submit a Jupyter Notebook named `CSC8851_F2025_HW3_<YourName>.ipynb` with all code and plots (runs top-to-bottom).
2. Submit a PDF export named `CSC8851_F2025_HW3_<YourName>.pdf`. Do not paste code screenshots. **Make sure your PDF version has the figures.**
3. Upload both files (`.ipynb` and `.pdf`) to iCollege.

You may include additional qualitative results (e.g., failure cases). Cite any external sources used.



(a) DDPM + CFG ($s = 2.0$).



(b) DDIM(50, $\eta=0$) + CFG ($s = 2.0$).

Figure 4: Conditional sampling results (rows: digits 0–9; 8 samples each).

Appendix: DDIM Sampling Details and Speed

Setup. Let $\alpha_t = 1 - \beta_t$ and $\bar{\alpha}_t = \prod_{i=0}^t \alpha_i$. Given a denoiser that predicts either $\hat{\mathbf{x}}_0(\mathbf{x}_t, t)$ or noise $\hat{\epsilon}(\mathbf{x}_t, t)$, we can convert between the two via

$$\hat{\epsilon}(\mathbf{x}_t, t) = \frac{\mathbf{x}_t - \sqrt{\bar{\alpha}_t} \hat{\mathbf{x}}_0}{\sqrt{1 - \bar{\alpha}_t}}, \quad \hat{\mathbf{x}}_0(\mathbf{x}_t, t) = \frac{\mathbf{x}_t - \sqrt{1 - \bar{\alpha}_t} \hat{\epsilon}}{\sqrt{\bar{\alpha}_t}}. \quad (1)$$

DDPM vs. DDIM (one-step updates)

DDPM (Markovian, stochastic). A common parameterization of the reverse step is

$$\mathbf{x}_{t-1}^{(\text{DDPM})} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1 - \bar{\alpha}_t}} \hat{\epsilon}(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}, \quad \mathbf{z} \sim \mathcal{N}(0, \mathbf{I}), \quad (2)$$

where σ_t^2 is chosen from the DDPM posterior variance family. This update is *Markovian* and typically run at all T steps (e.g., $T=1000$).

DDIM (non-Markovian, implicit). DDIM defines a family of trajectories that share the same single-step marginals as DDPM but allow skipping steps and optionally removing noise. For a chosen subsequence of indices

$$\mathcal{S} = \{\tau_1 > \tau_2 > \dots > \tau_K\}, \quad K \ll T,$$

the DDIM step from τ_k to τ_{k+1} is

$$\sigma_{\tau_k}^{(\text{DDIM})} = \eta \sqrt{\frac{1 - \bar{\alpha}_{\tau_{k+1}}}{1 - \bar{\alpha}_{\tau_k}}} \sqrt{1 - \frac{\bar{\alpha}_{\tau_k}}{\bar{\alpha}_{\tau_{k+1}}}}, \quad (3)$$

$$\mathbf{x}_{\tau_{k+1}}^{(\text{DDIM})} = \sqrt{\bar{\alpha}_{\tau_{k+1}}} \hat{\mathbf{x}}_0 + \sqrt{1 - \bar{\alpha}_{\tau_{k+1}} - (\sigma_{\tau_k}^{(\text{DDIM})})^2} \hat{\epsilon} + \sigma_{\tau_k}^{(\text{DDIM})} \mathbf{z}, \quad \mathbf{z} \sim \mathcal{N}(0, \mathbf{I}), \quad (4)$$

with $\hat{\mathbf{x}}_0$ and $\hat{\epsilon}$ evaluated at $(\mathbf{x}_{\tau_k}, \tau_k)$ and related by (1). The hyperparameter $\eta \in [0, 1]$ controls stochasticity.

Deterministic DDIM (fast default). Setting $\eta = 0$ yields

$$\mathbf{x}_{\tau_{k+1}} = \sqrt{\bar{\alpha}_{\tau_{k+1}}} \hat{\mathbf{x}}_0 + \sqrt{1 - \bar{\alpha}_{\tau_{k+1}}} \hat{\boldsymbol{\epsilon}} \quad (\eta = 0). \quad (5)$$

No per-step noise is injected; the trajectory becomes a deterministic mapping guided by the denoiser.

Where the speed-up comes from

- **Fewer model calls.** DDPM typically uses all T small steps. DDIM chooses a *coarse* timestep set \mathcal{S} (e.g., $K=50$) and updates using (4). Complexity drops from $\mathcal{O}(T)$ to $\mathcal{O}(K)$ denoiser evaluations (e.g., $\sim 20\times$ fewer if $K=50, T=1000$).
- **Stable large steps.** Because the DDIM update directly re-targets the next marginal with the pair $(\bar{\alpha}_{\tau_k}, \bar{\alpha}_{\tau_{k+1}})$ and the predicted $(\hat{\mathbf{x}}_0, \hat{\boldsymbol{\epsilon}})$, it tolerates larger jumps in t than the stochastic DDPM posterior step.
- **Optional determinism.** With $\eta=0$ (Eq. (5)), trajectories are noise-free and invertible in the ideal case, which improves consistency at small K and further reduces sampling variance.

DDPM Generation (Pseudocode)

Algorithm: DDPM Sampling (x0-prediction) with optional CFG

Inputs:

- Trained model that predicts x0: `x0_hat = model(Z, t).sample`
- Labels `y (B,)`, image shape `(B,1,H,W)` with $H=W=32$ for MNIST
- Full timestep set `S_full = {T-1, ..., 0}` (usually $T=1000$)
- Guidance scale `s >= 0` (use `s=0` to disable CFG)
- Precomputed `alpha[t]`, `alpha_bar[t]`, and posterior variance `tilde_beta[t]`

Initialize:

```
X <- Normal(0, I)          # X has shape (B, 1, H, W)
```

```
for each t in S_full:      # reverse order: T-1, T-2, ..., 0
```

```
  # ----- (A) Predict x0 (conditional + unconditional for CFG) -----
```

```
  Zc <- concat(X, class_maps(y))          # (B, 11, H, W)
```

```
  x0_cond <- model(Zc, t).sample          # \hat{x}_0^{cond}
```

```
  Zu <- concat(X, zeros_like(class_maps(y))) # unconditional input
```

```
  x0_uncond <- model(Zu, t).sample        # \hat{x}_0^{uncond}
```

```
  x0_hat <- x0_cond + s * (x0_cond - x0_uncond) # CFG combine (s=0 disables)
```

```
  # ----- (B) Convert \hat{x}_0 -> predicted noise \hat{\epsilon} (optional) -----
```

```
  eps_hat <- (X - sqrt(alpha_bar[t]) * x0_hat) / sqrt(1 - alpha_bar[t])
```

```

# ----- (C) DDPM update (two equivalent forms) -----

# Form 1: noise-parameterized mean + stochasticity
mu = (1 / sqrt(alpha[t])) * (X - (1 - alpha[t]) / sqrt(1 - alpha_bar[t]) * eps_hat)
sigma = sqrt(tilde_beta[t]) # posterior std (DDPM original choice)
X_prev = mu + sigma * Normal(0, I)

# Form 2: x0/epsilon mixture (algebraically equivalent)
# c = sqrt(1 - alpha_bar[t-1] - tilde_beta[t]) # define c for convenience
# X_prev = sqrt(alpha_bar[t-1]) * x0_hat + c * eps_hat
#           + sqrt(tilde_beta[t]) * Normal(0, I)

X <- X_prev

# Output (denormalize as needed)
return X

```

Remarks.

- DDPM is *Markovian* and injects noise at every step via the posterior variance $\tilde{\beta}_t$ (or a scaled variant).
- In practice, we rarely hand-code μ and σ ; the scheduler computes the reverse step given \hat{x}_0 (or $\hat{\epsilon}$) and the current sample.

DDIM Generation (Pseudocode)

Algorithm: DDIM Sampling (x0-prediction) with optional CFG

Inputs:

- Trained model that predicts x0: $x0_hat = model(Z, t).sample$
- Labels y (B,), image shape (B, 1, H, W) with $H=W=32$ for MNIST
- Short timestep set $S = \{\tau_1 > \tau_2 > \dots > \tau_K\}$, $K \ll T$ (e.g., $K=50$)
- Guidance scale $s \geq 0$ (use $s=0$ to disable CFG)
- DDIM stochasticity η in $[0, 1]$ (use $\eta=0$ for deterministic DDIM)
- Precomputed $\alpha_bar[t]$ for all t (cumulative product of alphas)

Initialize:

```
X <- Normal(0, I) # X has shape (B, 1, H, W)
```

for $k = 1$ to $K-1$:

```

t      <- tau_k
t_prev <- tau_{k+1}

```

```
# ----- (A) Predict x0 (conditional + unconditional for CFG) -----
```



```

Zc <- concat(X, class_maps(y))                # (B, 11, H, W)
x0_cond <- model(Zc, t).sample                  #  $\hat{x}_0^{\text{cond}}$ 

Zu <- concat(X, zeros_like(class_maps(y)))     # unconditional input
x0_uncond <- model(Zu, t).sample                #  $\hat{x}_0^{\text{uncond}}$ 

x0_hat <- x0_cond + s * (x0_cond - x0_uncond) # CFG combine (s=0 disables)

# ----- (B) Convert  $\hat{x}_0$  to predicted noise  $\hat{\epsilon}$  -----
eps_hat <- (X - sqrt(alpha_bar[t]) * x0_hat) / sqrt(1 - alpha_bar[t])

# ----- (C) DDIM variance and update -----
# sigma controls stochasticity of the step (DDIM general form):
sigma = eta
      * sqrt( (1 - alpha_bar[t_prev]) / (1 - alpha_bar[t]) )
      * sqrt( 1 - alpha_bar[t] / alpha_bar[t_prev] )

c = sqrt( 1 - alpha_bar[t_prev] - sigma^2 )

# DDIM step from t -> t_prev:
X_prev = sqrt(alpha_bar[t_prev]) * x0_hat
      + c * eps_hat
      + sigma * Normal(0, I)                    # drop this term if eta=0

X <- X_prev

# Output (denormalize for viewing as needed):
return X

```

Using diffusers: DDPM vs. DDIM (x_0 -prediction)

DDPM (full steps).

```

# Assume: model predicts x0 (prediction_type="sample")
ddpm.set_timesteps(ddpm.config.num_train_timesteps) # typically T=1000
X = Normal(0, I)                                     # (B,1,32,32)
for t in ddpm.timesteps:
    Zc = concat(X, class_maps(y))
    Zu = concat(X, zeros_like(class_maps(y)))
    x0_c = model(Zc, t).sample
    x0_u = model(Zu, t).sample
    x0_cfg = x0_c + s * (x0_c - x0_u)                # CFG combine
    step = ddpm.step(model_output=x0_cfg, timestep=t, sample=X)
    X = step.prev_sample
# X is the generated image batch

```

DDIM (short trajectory, optional determinism).

```
# Use far fewer steps (e.g., K=50) and optionally set eta=0 for deterministic DDIM
ddim.set_timesteps(K)                                # K << T, e.g., 50
X = Normal(0, I)                                       # (B,1,32,32)
for t in ddim.timesteps:
    Zc = concat(X, class_maps(y))
    Zu = concat(X, zeros_like(class_maps(y)))
    x0_c = model(Zc, t).sample
    x0_u = model(Zu, t).sample
    x0_cfg = x0_c + s * (x0_c - x0_u)                  # CFG combine
    step = ddim.step(model_output=x0_cfg, timestep=t, sample=X, eta=0.0)
    X = step.prev_sample
# X is the generated image batch
```

Key differences.

- **DDPM:** Markovian, stochastic reverse process, typically run for all T steps; higher compute cost.
- **DDIM:** Non-Markovian implicit update; can jump across a subset of timesteps $K \ll T$ and be deterministic ($\eta=0$), giving a large speed-up with comparable quality.

Notes.

- **Difference vs. DDPM.** DDPM uses a Markovian posterior update with per-step noise and is typically run for all T steps. DDIM uses a *non-Markovian* implicit update that can jump across a *subset* of steps \mathcal{S} (e.g., 50) and can be *deterministic* for $\eta = 0$.
- **Speed-up.** Reducing the number of denoiser calls from T to K yields $\mathcal{O}(T/K)$ speed-up (e.g., $1000 \rightarrow 50$ gives $\sim 20\times$ fewer steps) with competitive quality.
- **Disabling CFG.** Set $s = 0$ to use unconditional sampling (or provide only the conditional branch and set $x_0^{\text{uncond}} = 0$).
- **Shapes.** For MNIST: $X \in \mathbb{R}^{B \times 1 \times 32 \times 32}$, class maps $(B, 10, 32, 32)$, model input $Z \in \mathbb{R}^{B \times 11 \times 32 \times 32}$.