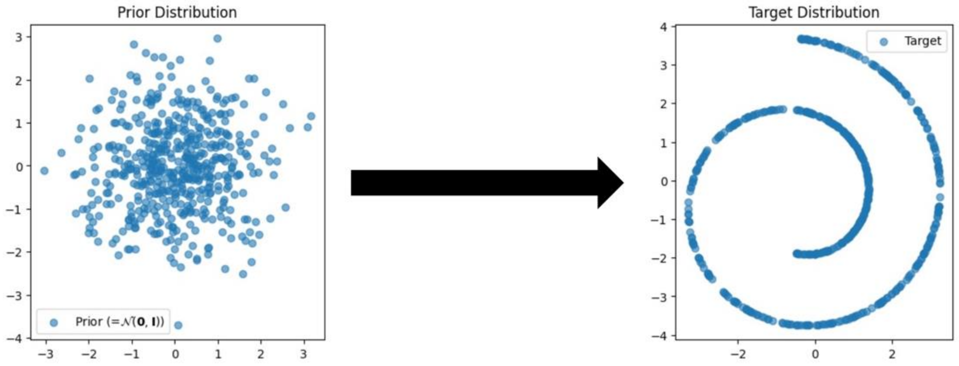
Lab 1 - DDPM



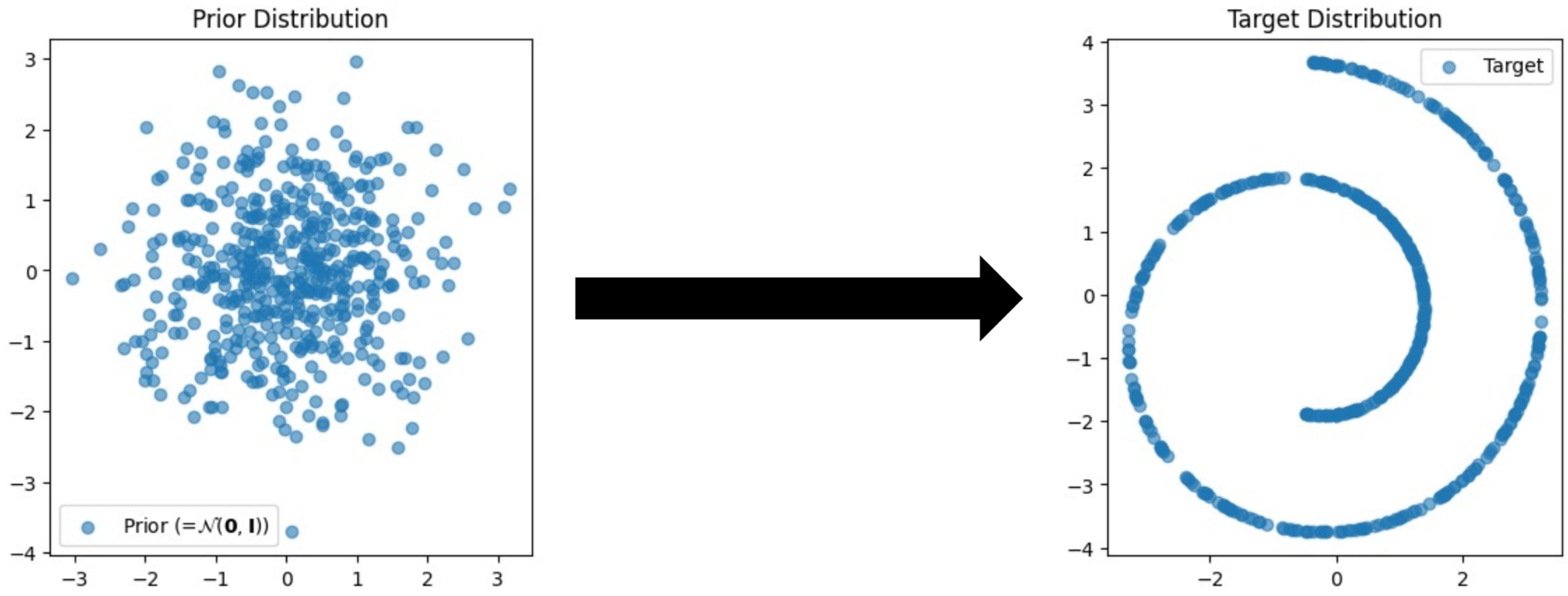
Task 1 - Swiss Roll

Task 2 - Image Generation

DDPM paper

Task 1 - Swiss Roll

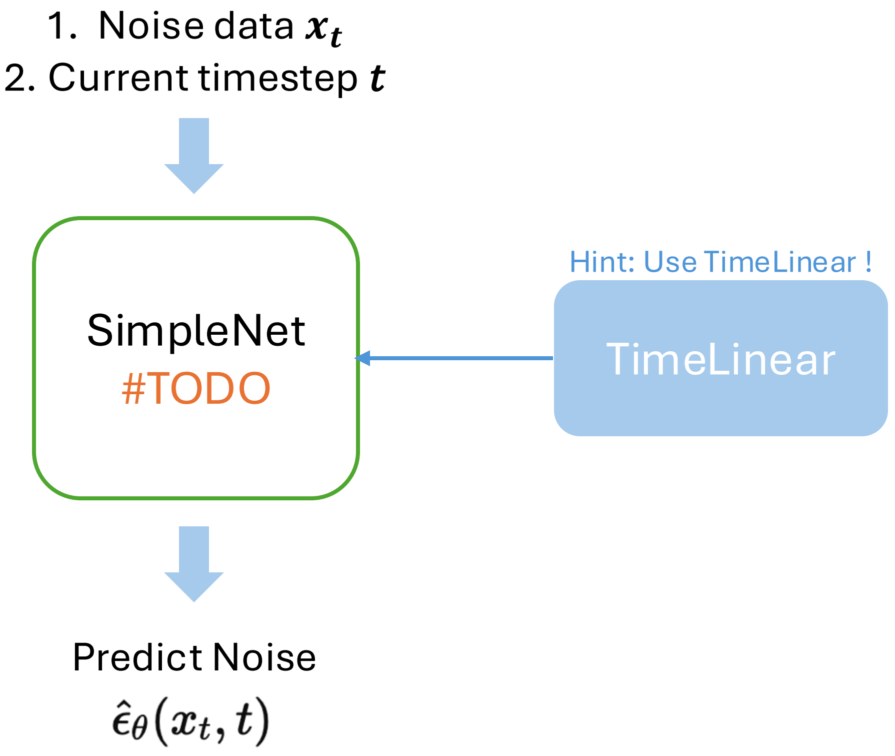
Let’s begin by modeling a simple distribution of 2D points (“Swiss Roll”).



Task 1

#TODO1 - SimpleNet

- 2d_plot_diffusion_todo/network.py

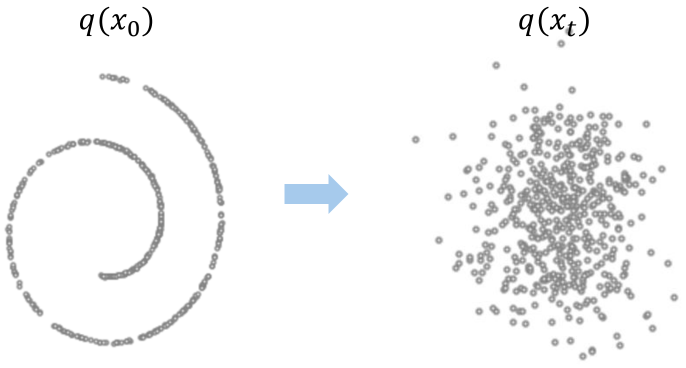



```python
class SimpleNet(nn.Module):
    def __init__(
        self, dim_in: int, dim_out: int, dim_hids: List[int], num_timesteps: int
    ):
        super().__init__()
        """
        (TODO) Build a noise estimating network.

        Args:
            dim_in: dimension of input
            dim_out: dimension of output
            dim_hids: dimensions of hidden features
            num_timesteps: number of timesteps
        """

        ######## TODO ########
        # DO NOT change the code outside this part.

        ######################

    def forward(self, x: torch.Tensor, t: torch.Tensor):
        """
        (TODO) Implement the forward pass. This should output
        the noise prediction of the noisy input x at timestep t.

        Args:
            x: the noisy data after t period diffusion
            t: the time that the forward diffusion has been running
        """
        ######## TODO ########
        # DO NOT change the code outside this part.

        ######################
        return x
```

Task 1

#TODO2 - q_sample

- 2d_plot_diffusion_todo/ddpm.py



$$q(x_t \mid x_0) = N(x_t; \sqrt{\bar{\alpha}_t}\, x_0, (1 - \bar{\alpha}_t) I).$$

```
def q_sample(self, x0, t, noise=None):
    """
    sample x_t from q(x_t | x_0) of DDPM.

    Input:
        x0 (`torch.Tensor`): clean data to be mapped to timestep t in the forward process of DDPM.
        t (`torch.Tensor`): timestep
        noise (`torch.Tensor`, optional): random Gaussian noise. if None, randomly sample Gaussian noise i
    Output:
        xt (`torch.Tensor`): noisy samples
    """
    if noise is None:
        noise = torch.randn_like(x0)

    ######## TODO ########
    # DO NOT change the code outside this part.
    # Compute xt.
    alphas_prod_t = extract(self.var_scheduler.alphas_cumprod, t, x0)
    xt = x0

    ######################

    return xt
```

Task 1

#TODO2 - q_sample

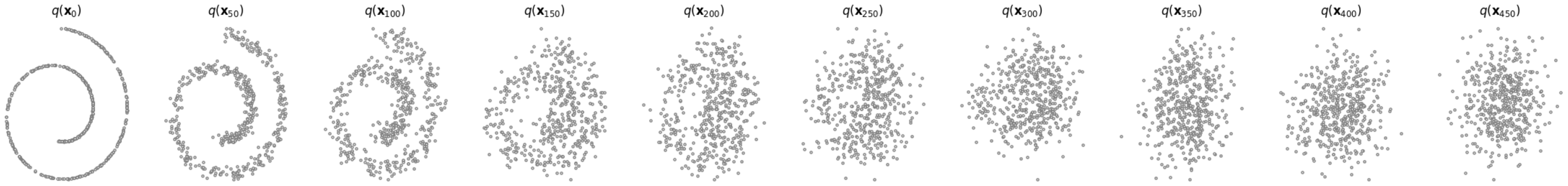
- 2d_plot_diffusion_todo/ddpm_tutorual.py

Check your implementation of q_sample !

Visualize q(x_t)

```python
fig, axs = plt.subplots(1, 10, figsize=(28, 3))
for i, t in enumerate(range(0, 500, 50)):
    x_t = ddpm.q_sample(target_ds[:num_vis_particles].to(device), (torch.ones(num_vis_par
    x_t = x_t.cpu()
    axs[i].scatter(x_t[:,0], x_t[:,1], color='white',edgecolor='gray', s=5)
    axs[i].set_axis_off()
    axs[i].set_title('$q(\mathbf{x}_{'+str(t)+'})$')
```

Python



Task 1

#TODO3 - p_sample

- 2d_plot_diffusion_todo/ddpm.py

How to get $x_t \xrightarrow{p_\theta} x_{t-1}$?

1. Predict noise from SimpleNet
2. $\mu_\theta(x_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\hat{\epsilon}_\theta(x_t, t)\right)$ **Eq. 11**
3. $\tilde{\beta}_t = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t$ **Sec. 3.2**
4. $x_{t-1} = \mu_\theta(x_t, t) + \sqrt{\tilde{\beta}_t}\, z, \quad z \sim \mathcal{N}(0, I)$ **Eq. 11**

```python
def p_sample(self, xt, t):
    """
    One step denoising function of DDPM: x_t -> x_{t-1}.
    Input:
        xt (`torch.Tensor`): samples at arbitrary timestep t.
        t (`torch.Tensor`): current timestep in a reverse process.
    Ouptut:
        x_t_prev (`torch.Tensor`): one step denoised sample. (= x_{t-1})
    """
    ######## TODO ########
    # DO NOT change the code outside this part.
    # compute x_t_prev.
    if isinstance(t, int):
        t = torch.tensor([t]).to(self.device)
    eps_factor = (1 - extract(self.var_scheduler.alphas, t, xt)) / (
        1 - extract(self.var_scheduler.alphas_cumprod, t, xt)
    ).sqrt()

    beta_t       = extract(self.var_scheduler.betas,          t, xt)       # β_t
    alpha_t      = extract(self.var_scheduler.alphas,         t, xt)       # α_t =
    alpha_bar_t = extract(self.var_scheduler.alphas_cumprod,  t, xt)       # \bar{
    t_prev       = (t - 1).clamp(min=0)
    alpha_bar_t_prev = extract(self.var_scheduler.alphas_cumprod, t_prev, xt) # \bar

    # 1. predict noise

    # 2. Posterior mean

    # 3. Posterior variance

    # 4. Reverse step

    #######################
    return x_t_prev
```

Task 1

#TODO4 - p_sample loop

- 2d_plot_diffusion_todo/ddpm.py

```python
def p_sample_loop(self, shape):
    """
    The loop of the reverse process of DDPM.

    Input:
        shape (`Tuple`): The shape of output. e.g., (num particles, 2)
    Output:
        x0_pred (`torch.Tensor`): The final denoised output through the DDPM reverse process.
    """
    ######## TODO ########
    # DO NOT change the code outside this part.
    # sample x0 based on Algorithm 2 of DDPM paper.
    x0_pred = torch.zeros(shape).to(self.device)

    ######################
    return x0_pred
```

Task 1

#TODO5 - compute_loss

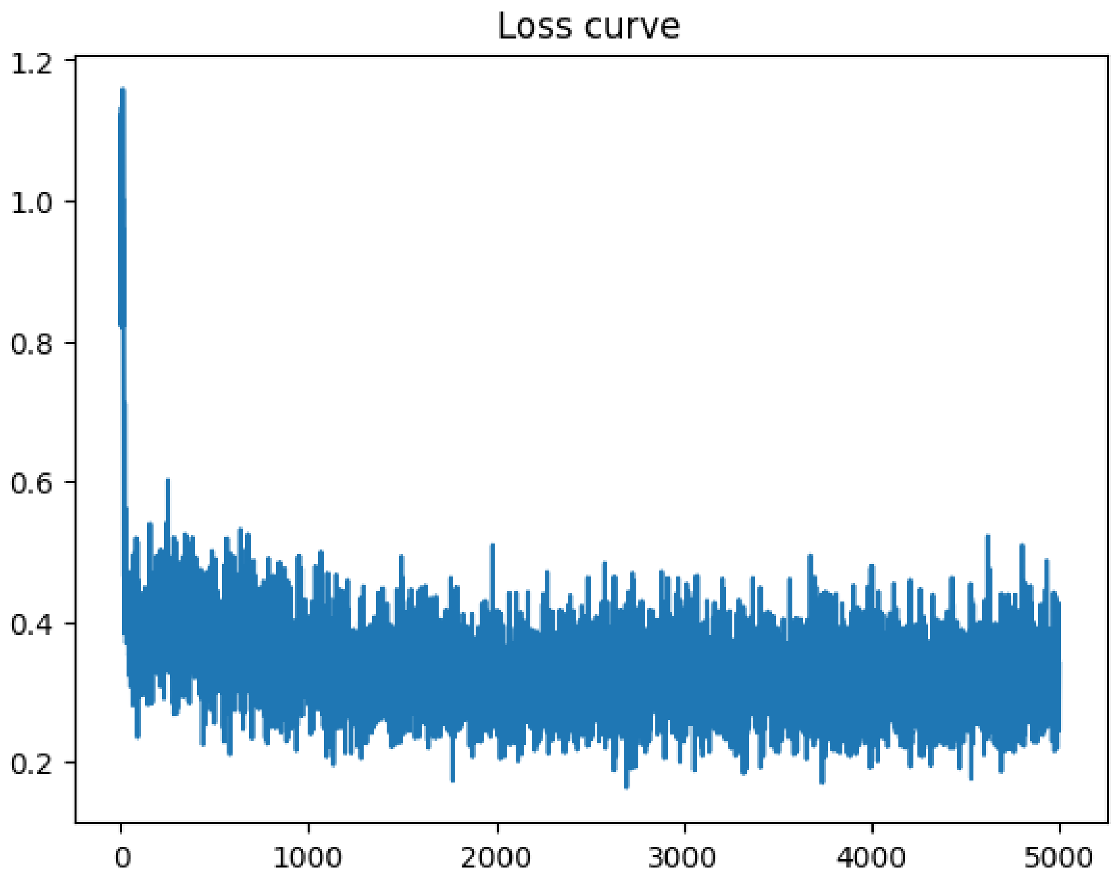
- 2d_plot_diffusion_todo/ddpm.py

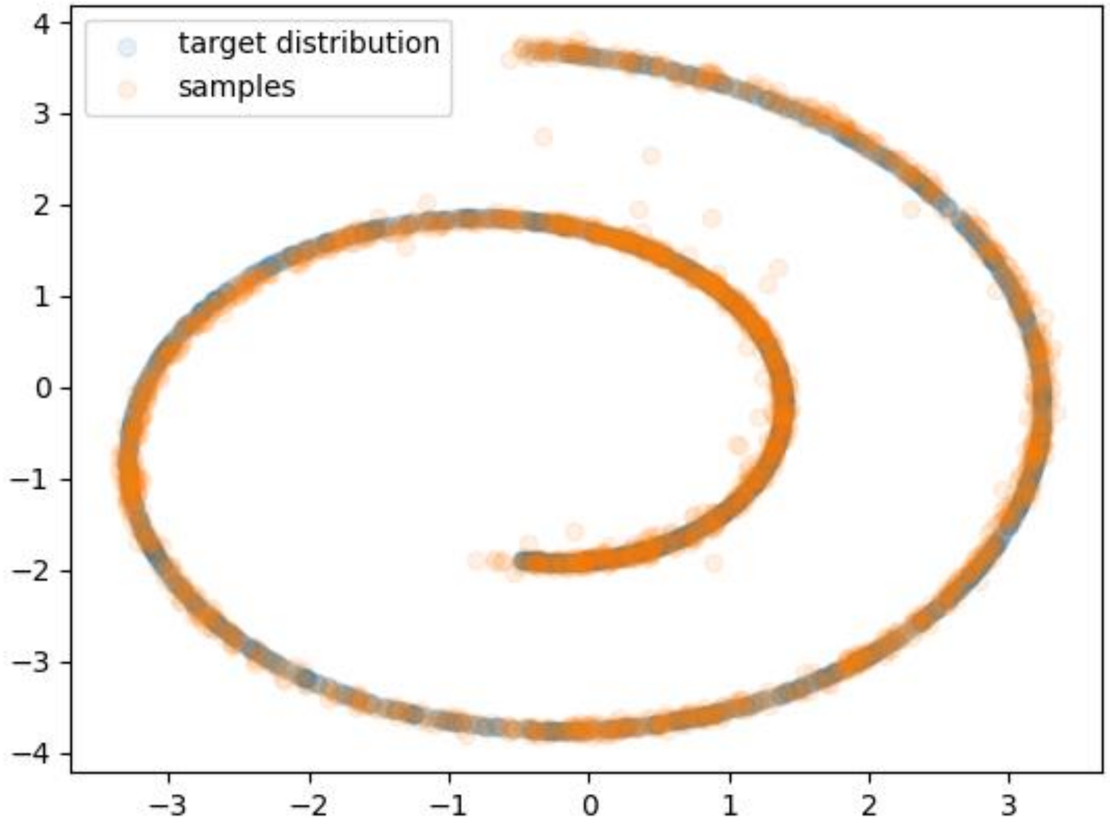
```python
def compute_loss(self, x0):
    """
    The simplified noise matching loss corresponding Equation 14 in DDPM paper.
    Input:
        x0 (`torch.Tensor`): clean data
    Output:
        loss: the computed loss to be backpropagated.
    """
    ######## TODO ########
    # DO NOT change the code outside this part.
    # compute noise matching loss.
    batch_size = x0.shape[0]

    # 1) random choose timestep
    t = (
        torch.randint(0, self.var_scheduler.num_train_timesteps, size=(batch_size,))
        .to(x0.device)
        .long()
    )
    # 2) get GT noise, and use q_sample to get x_t

    # 3) predict noise

    # 4) MSE loss (eps, eps_pred)

    loss = x0.mean()

    ######################
    return loss
```

Task 1

#TODO5 – train & evaluate

- 2d_plot_diffusion_todo/ddpm_tutorial.py

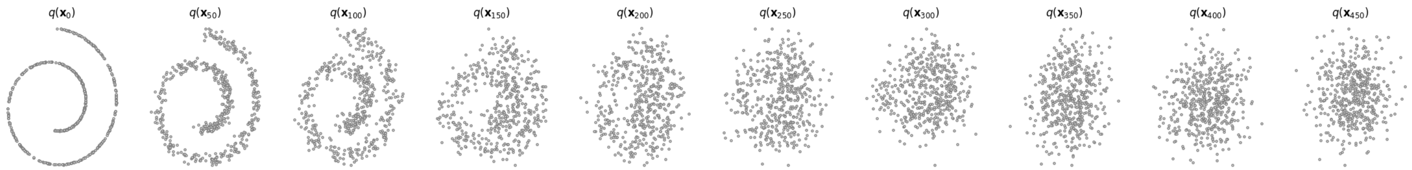




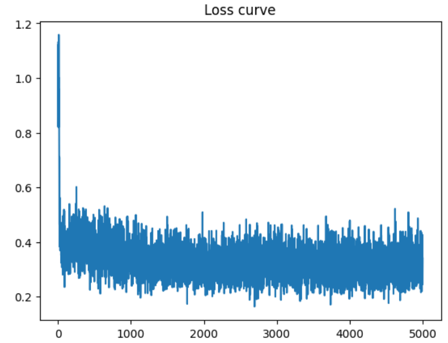
Task 1

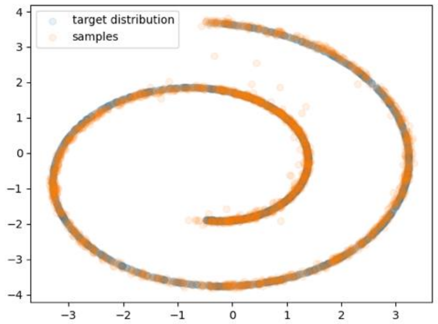
#Report

1. Write and Explain of all **#TODO** code (20pts)
2. Fig of your implementation of q_sample (10pts)



3. Fig of loss curve and evaluation result (10 pts)





Task 2 – Image Generation

What to Do: Task 2

Ugh...
Time to write more code...

Samples from our model trained using the AFHQ dataset.

Bring your codes from Task 1!

The code needs to be modified, but the changes should be kept minimal.

- q_sample → add_noise;
- p_sample → step;
- compute_loss → get_loss.

Task 2

TODO1 – add_noise

- image_diffusion_todo/scheduler.py

```
def add_noise(
    self,
    x_0: torch.Tensor,
    t: torch.IntTensor,
    eps: Optional[torch.Tensor] = None,
):
    """
    A forward pass of a Markov chain, i.e., q(x_t | x_0).

    Input:
        x_0 (`torch.Tensor [B,C,H,W]`): samples from a real data distribution q(x_0).
        t: (`torch.IntTensor [B]`)
        eps: (`torch.Tensor [B,C,H,W]`, optional): if None, randomly sample Gaussian noise in the function.
    Output:
        x_t: (`torch.Tensor [B,C,H,W]`): noisy samples at timestep t.
        eps: (`torch.Tensor [B,C,H,W]`): injected noise.
    """

    if eps is None:
        eps       = torch.randn(x_0.shape, device='cuda')

    ######## TODO ########
    # DO NOT change the code outside this part.
    # Assignment 1. Implement the DDPM forward step.
    x_t = None


    #######################

    return x_t, eps
```

Hint : Refer to 2d_plot_diffusion_todo/ddpm.py – **q_sample**

Task 2

TODO4 – beta scheduling

- image_diffusion_todo/scheduler.py

We know

$$q(x_t \mid x_0) = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t}\, \epsilon, \quad \epsilon \sim \mathcal{N}(0, I)$$

and

$$\alpha_t = 1 - \beta_t$$

$$\bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$$

Implement the **cosine scheduler**.

```python
if mode == "linear":
    betas = torch.linspace(beta_1, beta_T, steps=num_train_timesteps)
elif mode == "quad":
    betas = (
        torch.linspace(beta_1**0.5, beta_T**0.5, num_train_timesteps) ** 2
    )
elif mode == "cosine":
    ######## TODO ########
    # Implement the cosine beta schedule (Nichol & Dhariwal, 2021).
    # Hint:
    # 1. Define alphā_t = f(t/T) where f is a cosine schedule:
    #       alphā_t = cos^2( (t/T + s) / (1+s) ) * (π/2) )
    #    with s = 0.008 (a small constant for stability).
    # 2. Convert alphā_t into betas using:
    #       beta_t = 1 − alphā_t / alphā_{t-1}
    # 3. Return betas as a tensor of shape [num_train_timesteps].
    raise NotImplementedError("TODO: Implement cosine beta schedule here!")
```

Task 2

TODO5 – predictor

- image_diffusion_todo/scheduler.py

Implement the **reverse step** according to the chosen predictor (noise, x_0, or mean).

```python
def step_predict_noise(self, x_t: torch.Tensor, t: int, eps_theta: torch.Tensor):
    """
    Noise prediction version (the standard DDPM formulation).

    Input:
        x_t: noisy image at timestep t
        t: current timestep
        eps_theta: predicted noise ε̂_θ(x_t, t)
    Output:
        sample_prev: denoised image sample at timestep t-1
    """
    ######## TODO ########
    # 1. Extract beta_t, alpha_t, and alpha_bar_t from the scheduler.
    # 2. Compute the predicted mean μ_θ(x_t, t) = 1/√α_t * (x_t - (β_t/√(1-ᾱ_t)) *
    # 3. Compute the posterior variance \tilde{β}_t = ((1-ᾱ_{t-1})/(1-ᾱ_t)) * β_t.
    # 4. Add Gaussian noise scaled by √(\tilde{β}_t) unless t == 0.
    # 5. Return the final sample at t-1.
    sample_prev = None
    #######################
    return sample_prev
```

```python
def step_predict_x0(self, x_t: torch.Tensor, t: int, x0_pred: torch.Tensor):
    """
    x0 prediction version (alternative DDPM objective).

    Input:
        x_t: noisy image at timestep t
        t: current timestep
        x0_pred: predicted clean image x̂₀(x_t, t)
    Output:
        sample_prev: denoised image sample at timestep t-1
    """
    ######## TODO ########

    sample_prev = None
    #######################
    return sample_prev


def step_predict_mean(self, x_t: torch.Tensor, t: int, mean_theta: torch.Tensor):
    """
    Mean prediction version (directly outputting the posterior mean).

    Input:
        x_t: noisy image at timestep t
        t: current timestep
        mean_theta: network-predicted posterior mean μ̂_θ(x_t, t)
    Output:
        sample_prev: denoised image sample at timestep t-1
    """
    ######## TODO ########

    sample_prev = None
    #######################
    return sample_prev
```

Task 2

TODO5 – predictor

- image_diffusion_todo/model.py

Implement loss functions for training the network
to predict different targets: **noise**, **x_0**, or the **posterior mean**.

```python
def get_loss(self, x0, class_label=None, noise=None):
    if self.predictor == "noise":
        return self.get_loss_noise(x0, class_label, noise)
    elif self.predictor == "x0": #### TODO
        return self.get_loss_x0(x0, class_label, noise)
    elif self.predictor == "mean": #### TODO
        return self.get_loss_mean(x0, class_label, noise)
    else:
        raise ValueError(f"Unknown predictor: {self.predictor}")
```

```python
def get_loss_x0(self, x0, class_label=None, noise=None):
    ######## TODO ########
    # Here we implement the "predict x0" version.
    # 1. Sample a timestep and add noise to get (x_t, noise).
    # 2. Pass (x_t, timestep) into self.network, where the output should represent the clean sample x0_pred.
    # 3. Compute the loss as MSE(predicted x0_pred, ground-truth x0).
    ######################
    loss = None
    return loss

def get_loss_mean(self, x0, class_label=None, noise=None):
    ######## TODO ########
    # Here we implement the "predict mean" version.
    # 1. Sample a timestep and add noise to get (x_t, noise).
    # 2. Pass (x_t, timestep) into self.network, where the output should represent the posterior mean μθ(x_t, t)
    # 3. Compute the *true* posterior mean from the closed-form DDPM formula (using x0, x_t, noise, and schedule
    # 4. Compute the loss as MSE(predicted mean, true mean).
    ######################
    loss = None
    return loss
```

Task 2

TODO5 - train

- image_diffusion_todo/train.py

python train.py --mode {BETA_SCHEDULING} --predictor {PREDICTOR}

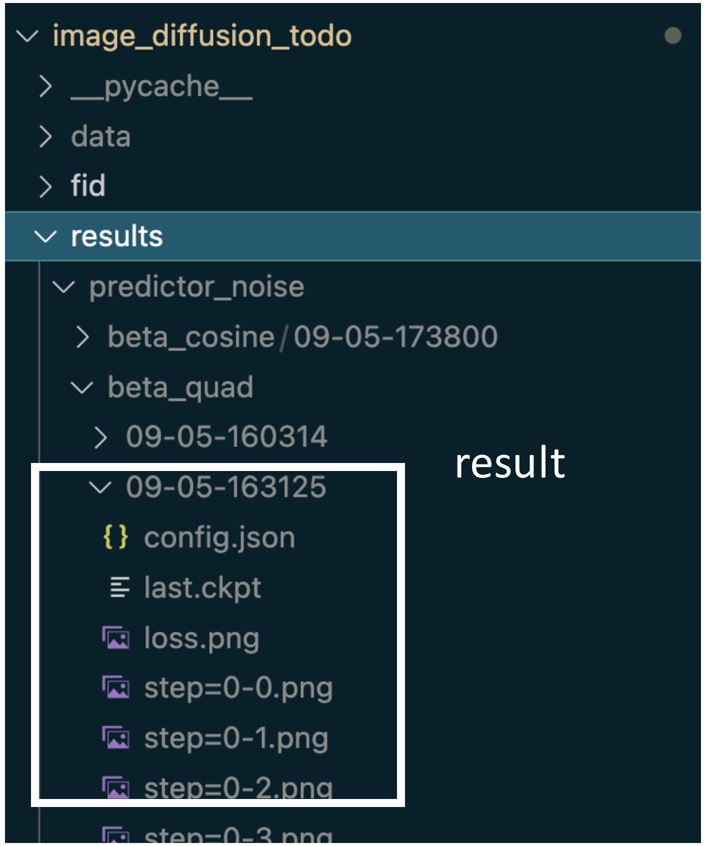
Try different **beta scheduling**:

1. linear
2. quadratic
3. cosine

Try different **predictor**:

1. noise (default)
2. mean
3. x_0

Please train for at least **50,000–100,000** iterations.
Training may take **over 6 hours per time**, so start ASAP!

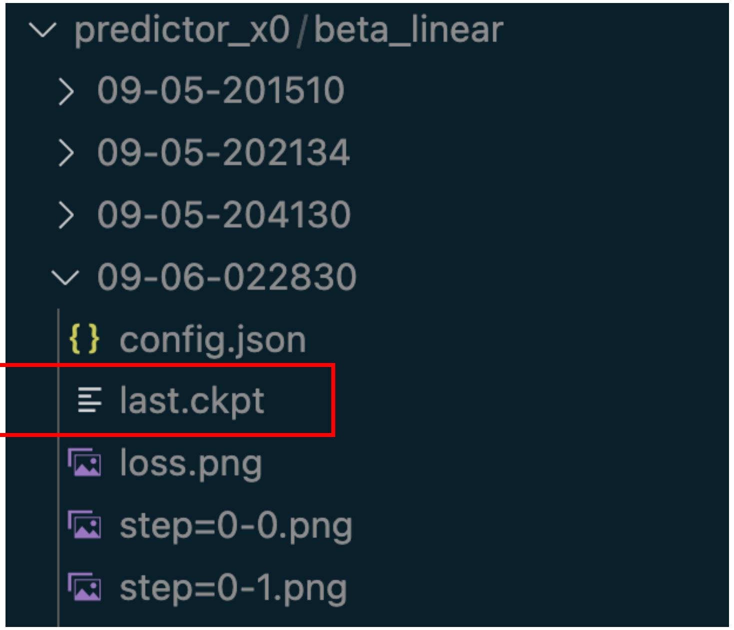


Task 2

TODO5 - sampling

- image_diffusion_todo/sampling.py

python sampling.py --ckpt_path {CKPT} --save_dir {SAVE}




```
num_train_timesteps = ddpm.var_scheduler.num_train_timesteps
ddpm.var_scheduler = DDPMScheduler(
    num_train_timesteps,
    beta_1=1e-4,
    beta_T=0.02,
    ### TODO ###
    mode="linear",  #cosine # quadratic
).to(device)
```

Remember to change the corresponding scheduler

Task 2

TODO5 - evaluate

- image_diffusion_todo/dataset.py

Prepare the data for evaluation by running

python dataset.py (Only once!)

This will create the eval directory under data/afhq.

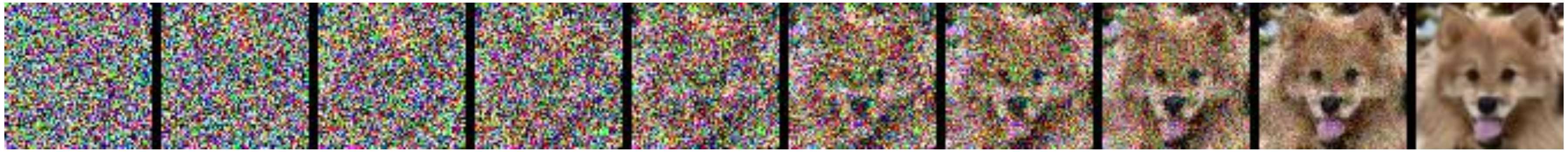
Do NOT forget to run this. Otherwise, you will get incorrect FIDs!

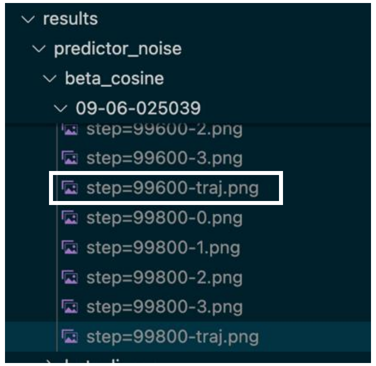
Task 2

#Report

1. Complete and Explain of all **#TODO** code. (30pts)
2. Show the **trajectory fig** and compare results across the three **beta schedulers**.

   (linear, quadratic, cosine) (10pts)





3. Show the results of different **predictors** (noise, x_0, posterior mean) and discuss. (10pts)

8 samples per predictor, 24 in total.

4. Screenshot of the **Best FID** of your training result, explain the training setting. (20pts)

- 20 pts: FID < 15
- 15 pts: 15 ≤ FID < 20
- 10 pts: 20 ≤ FID < 30
- 5 pts: 30 ≤ FID < 40
- 0 pts: FID ≥ 40

Submit

Create a single ZIP file {ID}_lab1.zip including:

- The **PDF** file formatted following the guideline;
- Your **code** without checkpoints for DDPMs and the Inception Network

412551014_lab1.zip

- report.pdf

- 2d_plot_diffusion_todo

- image_diffusion_todo

Thank you