Advanced Machine Learning

Unsupervised Representation Learning from Pre-trained Diffusion Probabilistic Models

by Zijian Zhang, Zhou Zhao and Zhijie Lin

Maziane Yassine

Authors

Zijian Zhang : PhD student at Zhejiang University
Zhou Zhao : Associate Professor at Zhejiang University
Zhijie Lin : Researcher at Sea AI Lab

Publication journal

Paper was accepted at Advances in Neural Information Processing Systems 35 (NeurIPS 2022)

Context

The authors propose Pre-traine DPM AutoEncoding (PDAE), a variant of DPM where a latent z holding much information about the data is trained to allow :

- Better reconstruction and higher sample quality
- Learning meaningful representations of the data

Background

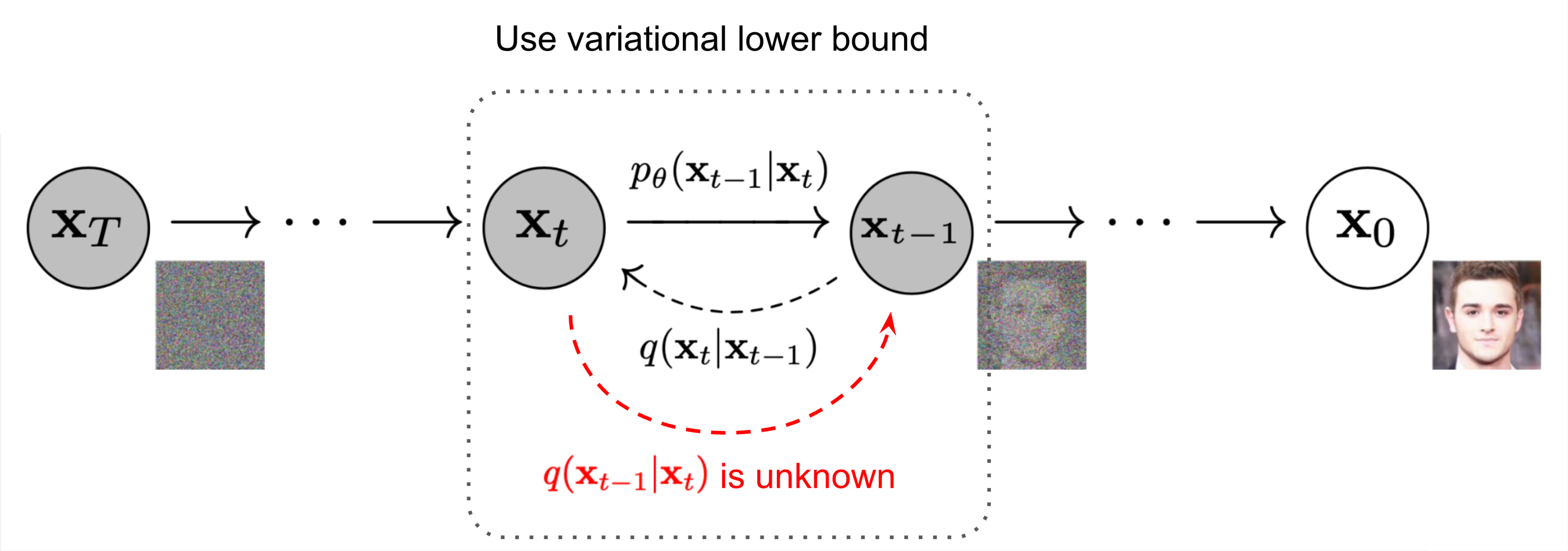
Diffusion Probabilistic Models : big picture

Diffusion models aim at learning the reverse of the noise generation procedure :

- Forward process : Add noise to the original sample x_0 such that converges to x_T gaussian
- Backward process : Recover the original sample from the noise

Background

Diffusion Probabilistic Models : big picture



source : "https://lilianweng.github.io/posts/2021-07-11-diffusion-models/"

Background

Diffusion Probabilistic Models : Markov chains definition

The forward process is defined by :
$q(x_t|x_{t-1}) = N(x_t; \mu_t = (1-\beta_t)x_{t-1}, \Sigma_t = \beta_t I)$

The backward process is defined by :
$p_\theta(x_{t-1}|x_t) = N(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$

Ideally we would like our model $p_\theta(x_{t-1}|x_t)$to exactly learn the distribution $q(x_{t-1}|x_t)$ but it is intractable by Bayes.

Background

Diffusion Probabilistic Models : training

What loss to use between distributions ? KL divergence

Loss : $E_q[D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t))]$

Or equivalently

$$E_{x_0,\epsilon,t}[||\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t)||^2]$$

Background

Classifier-guided Diffusion Probabilistic Models

- Classical DPM's : low control on the generated sample
- Classifier-guided DPM : high control of the class of the generated sample
  Simply push the sample towards high-density region $p(y|x_t)$.

$$p_\theta(x_{t-1}|x_t) = N(x_{t-1}; \mu_\theta(x_t, t) + \Sigma_\theta(x_t, t) \cdot \nabla_{x_t} \log p(y|x_t), \Sigma_\theta(x_t, t))$$

Background

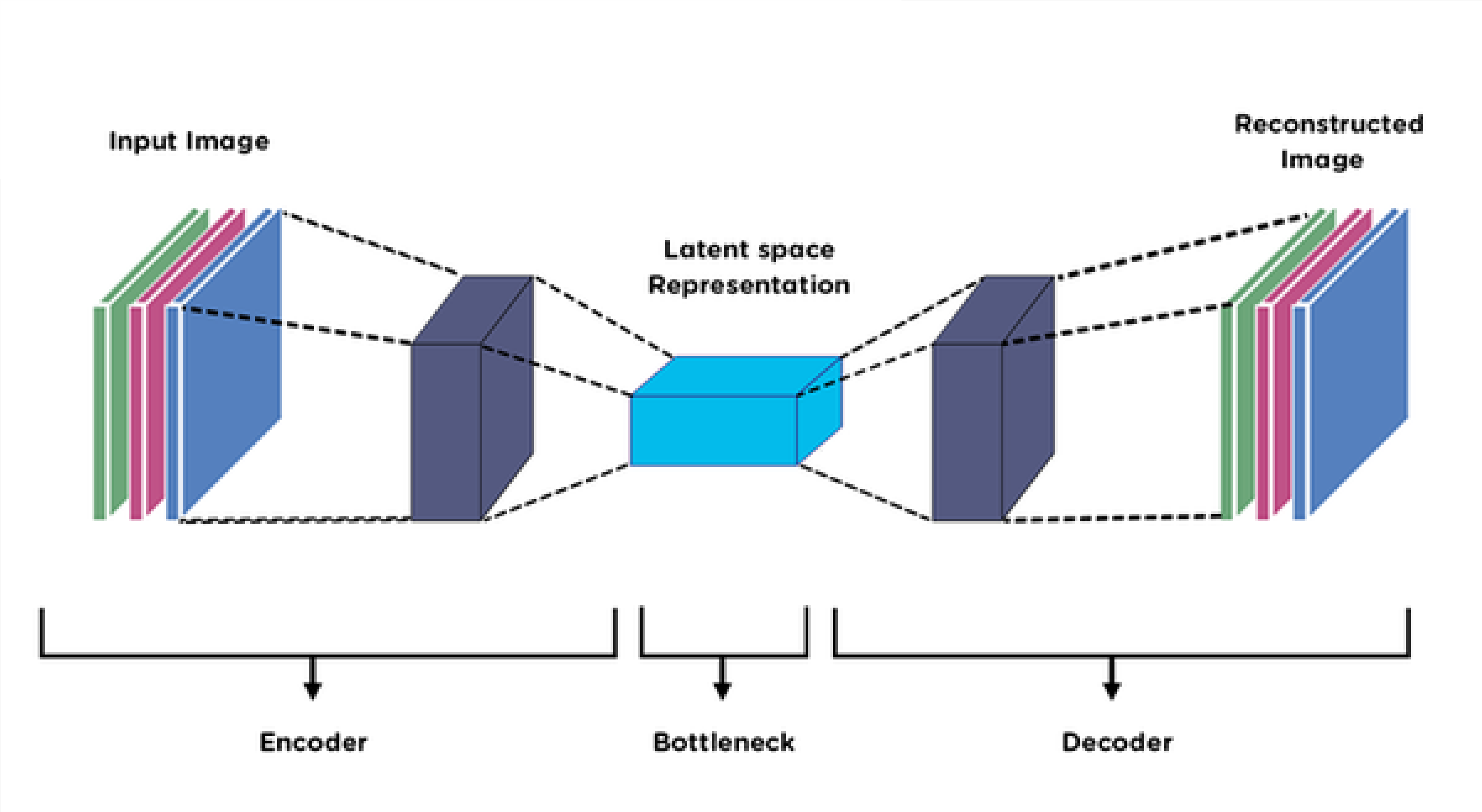
Autoencoders

Autoencoders: Unsupervised learning for efficient data representation

- Neural network architecture for learning compact representations
- Consists of an encoder and a decoder
- Encoder maps input data to a lower-dimensional latent space
- Decoder reconstructs the original input from the latent representation

Background

Autoencoders



Background

Representation Learning

- Extraction and construction of useful representations or features from raw data
- Aims to discover underlying structures and dependencies in the data
- Let the model learn these representations directly from the data rather than relying on handcrafted features designed by humans.

Paper observation

Authors observed that when diffusing an image and then denoising it, the reconstruction was never perfect regardless of the diffusion time or stochasticity involved, however, the reconstruction could be **improved** by using a **conditionnal** diffusion model.

Class information benefit

It seems the conditionnal gap is smaller than the unconditionnal gap

$$|\mu_\theta(x_t, y, t) - \tilde{\mu_\theta}(x_t, x_0)| \leq |\mu_\theta(x_t, t) - \tilde{\mu_\theta}(x_t, x_0)|$$

And they also observed the better reconstruction experimentally !

Essentially training is about injecting noise and removing it given (x_t, y, t)

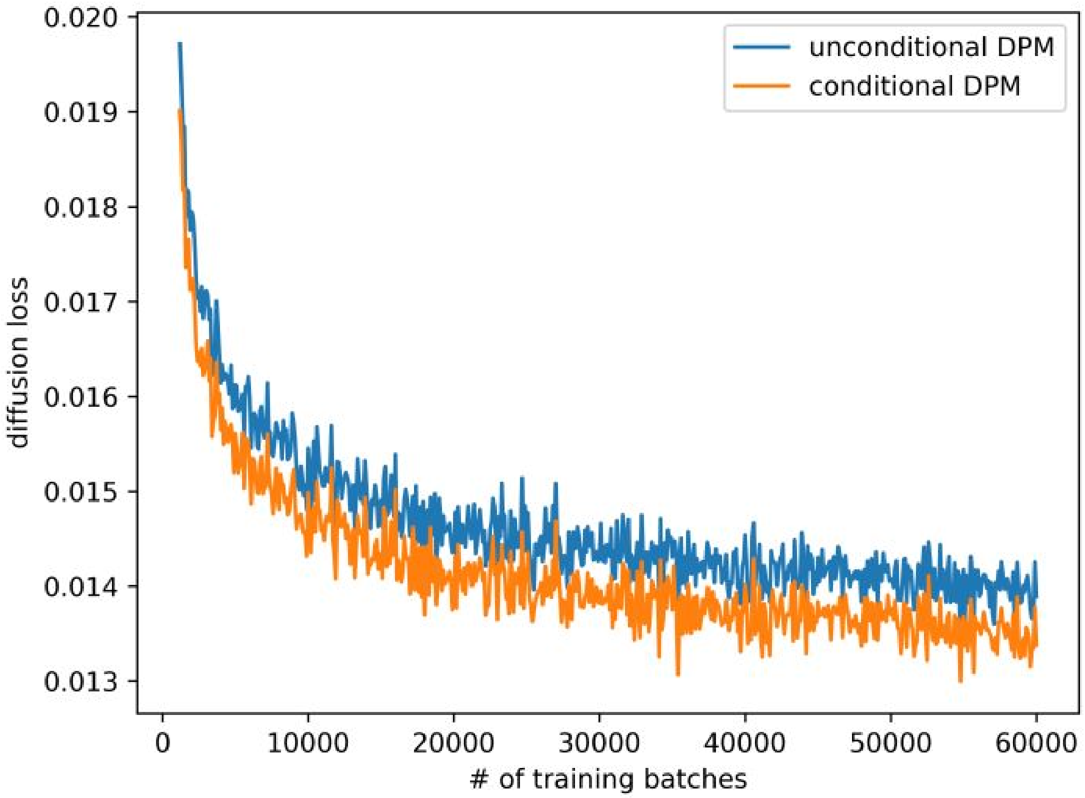


Figure 1: Comparison of diffusion loss between unconditional and conditional DPM trained on MNIST [28].

Class information benefit : WHY?

- Why can't unconditionnal DPM's have perfect reconstruction ?
- Why does the class information help reconstruction ?

-->Ask the audience

Class information benefit : WHY?

- Question : Why can't unconditionnal DPM's have perfect reconstruction ?
  Answer : Reconstruction is never perfect because the forward process **destroys** information. "Temporal latent variables lack high-level semantic information because they are just a sequence of spatially corrupted images."
- Question : why does the class information help reconstruction ?
  Answer : Simply because the class label is a **huge semantic information**

Information summary

1. The class label helps filling the gap by shifting the predicted mean by an item $\Sigma_\theta(x_t, t) \cdot \nabla_{x_t} \log p(y|x_t)$.
2. Even with the class label, reconstruction is not perfect because y does not capture the whole information of x_0.
3. In theory, if y contained all information of x_0, the gap could be fully filled and the reconstruction would be perfect

Main idea and contribution of the paper

Instead of using class information to fill the gap, **couldn't we inversely extract information about x_0 from the gap** ?
Instead of using y to fill the gap, couldn't we look for the best information summary $z = f(x_0)$ such that the gap is as small as possible ?
If z contains all information about x_0, the gap will be fully filled and the reconstruction perfect ... but this goes in the opposite direction as well !

Maths behind

Let E_ϕ be an AutoEncoder such that $z = E_\phi(x_0)$ and p_θ a pre-trained DPM such that $p_\theta(x_{t-1}|x_t) = N(x_{t-1}, \mu_\theta(x_t, t), \Sigma_\theta(x_t, t)$.

The conditionnal-DPM is :
$p_{\theta,\psi,\phi}(x_{t-1}|x_t, z) = N(x_{t-1}, \mu_\theta(x_t, t) + \Sigma_\theta(x_t, t) \cdot G_\psi(x_t, z, t), \Sigma_\theta(x_t, t))$

Where $G_\psi(x_t, z, t)$ simulates $\nabla_{x_t} p(z|x_t)$ where $p(z|x_t)$ is an implicit classifier.

Training

Training = Find an encoder E_ϕ and a gradient estimator G_ψ such that the gap is minimal.

Both models need to be good thus both models are trained jointly with

$$L(\psi, \phi) = E_{x_0,t,\epsilon}[\lambda_t||\epsilon - \epsilon_\theta(x_t, t) + \frac{\sqrt{\alpha_t}\sqrt{1-\bar{\alpha}_t}}{\beta_t} \cdot \Sigma_\theta(x_t, t) \cdot G_\psi(x_t, E_\phi(x_0), t)||^2]$$

where $x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon$ and where λ_t is a new weighting scheme defined by the authors

Training

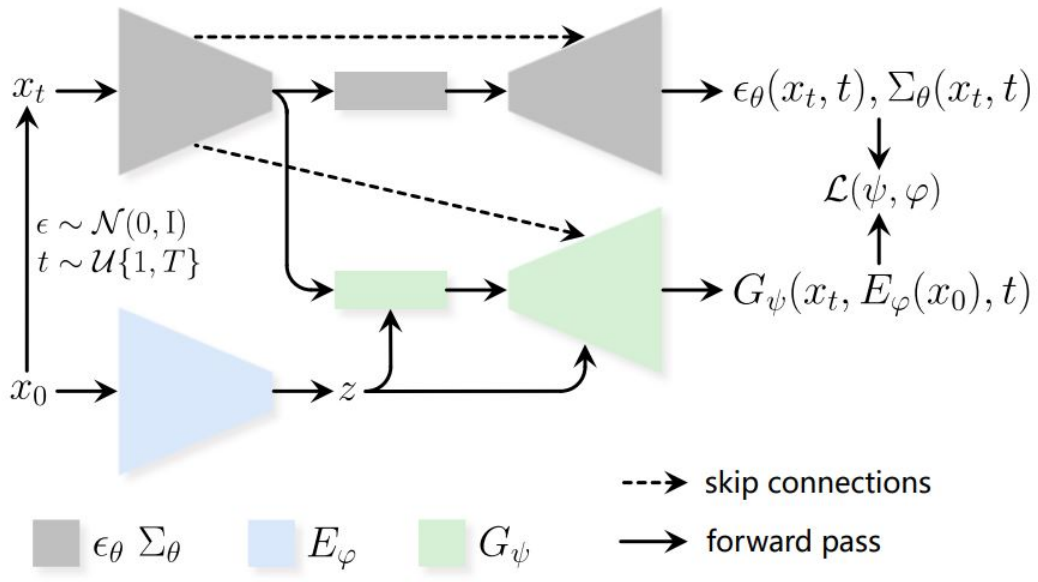


Figure 2: Network and data flow of PDAE. The gray part represents the pre-trained DPM, which is frozen during training.

$$L(\psi, \phi) = E_{x_0,t,\epsilon}[\lambda_t||\epsilon - \epsilon_\theta(x_t, t) + \frac{\sqrt{\alpha_t}\sqrt{1-\bar{\alpha}_t}}{\beta_t} \cdot \Sigma_\theta(x_t, t) \cdot G_\psi(x_t, E_\phi(x_0), t)||^2]$$

Network architecture

- E_ϕ is a simple CNN + 1 FC
- $G_\psi(x_t, z, t)$ is a U-Net similar to that of $\epsilon_\theta(x_t, t)$ which already takes x_t and t as inputs and thus we can leverage the knowledge of the trained DPM by using the time embedding layer and the encoder part of the U-Net such that in the end we only need to embed z.

Diffusion timesteps importance

For sample quality reasons, $\lambda_t = 1$ is most often used but authors made an interesting observation : some timesteps matter more than others. Consider the following mixed sampling procedure :

1. Unconditionally generate a sample from t = T -> $t = t_1$
2. Continue with classifier-guided diffusion from $t = t_1$ to $t = t_2$
3. Go back to unconditional diffusion

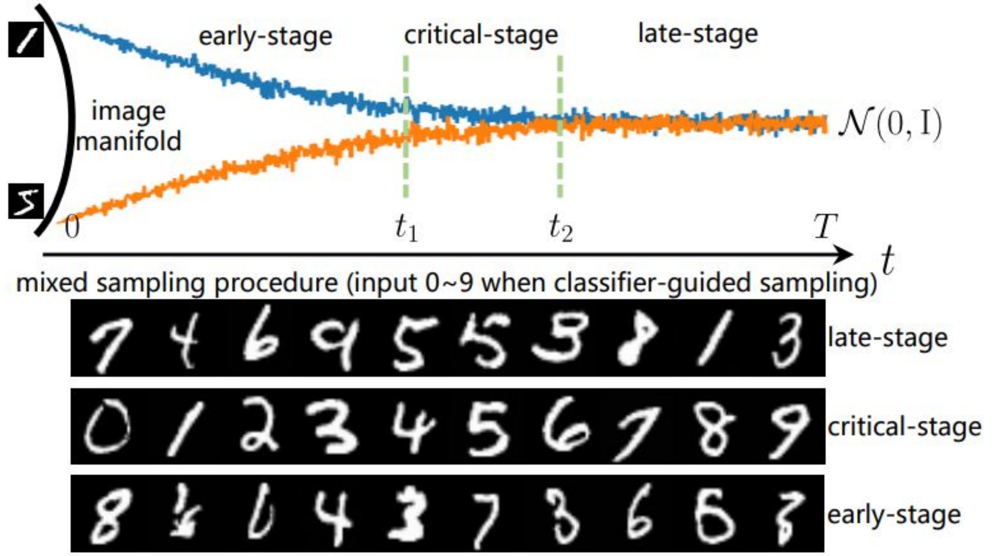


Figure 3: Investigations of the effects of mean shift for different time stages. We perform a 50-step-grid-search for (t_1, t_2) pairs to find the shortest critical-stage that can ensure high accuracy of conditional generation. For MNIST [28], it is $(400, 700)$.

"We can conclude that the mean shift during critical-stage contains more crucial information to reconstruct the input class label in samples than the other two stages"

Experiments

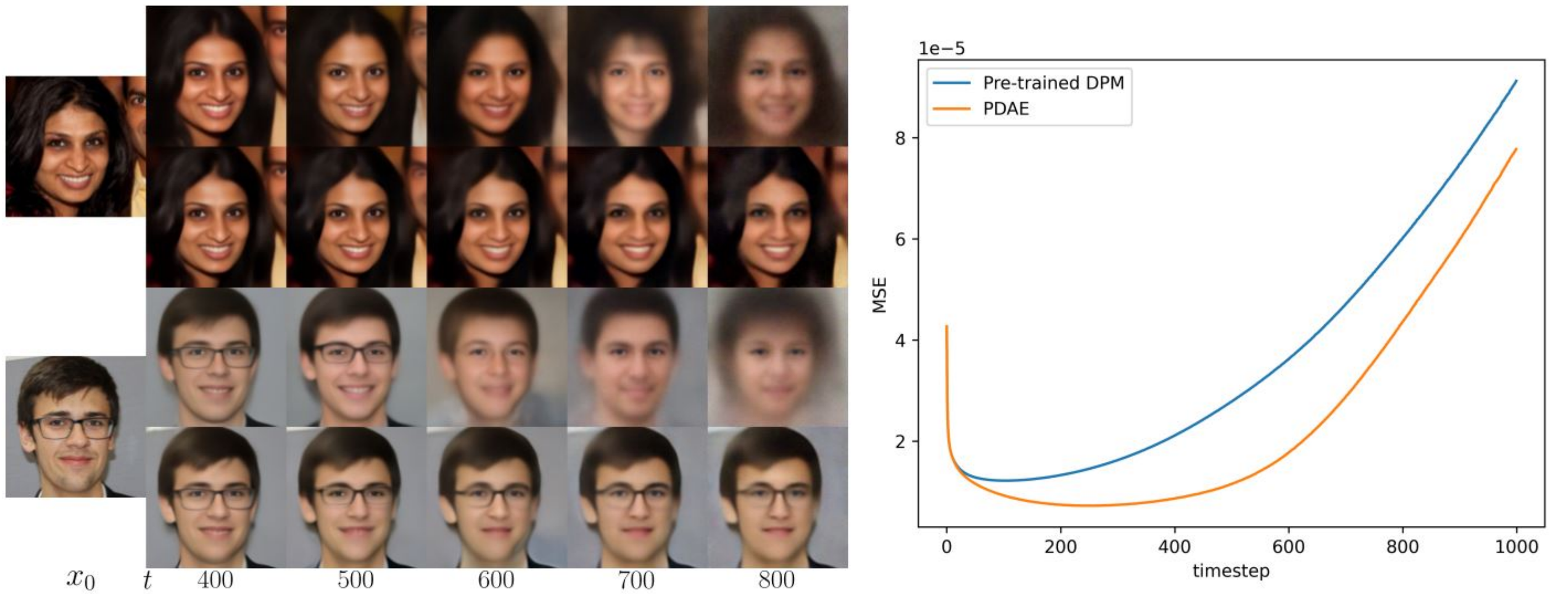


Figure 5: **Left**: Predicted $\hat{\boldsymbol{x}}_0$ by denoising $\boldsymbol{x}_t$ for only one step. The first row use pre-trained DPM and the second row use PDAE. **Right**: Average posterior mean gap for all steps.

The latent seems to bring quite a lot of information useful to reconstruction. ("FFHQ128-130M-z512-64M")

Critics

Pros

- Main concurrent work, diff-AE, had to retrain a whole DPM to achieve similar performance resulting in PDAE requiring 2 to 3 times less training batches.
- Managed to reach attribute manipulation
- Paper is simple to read
- Elegant main idea

Critics

Cons

- The approximated gradient G_ψ might be far from an actual gradient, it is simply there to provide a better noise prediction
- G_ψ architecture being more complex than E_ϕ, it might hide the defaults and quality of E_ϕ.
- The conclusion from the mixed samplings is strong, further evidence such as MSE according to the several (t_1, t_2) pairs would have been welcome
- There is no simple decoder as $E_\phi^- 1$

Critics

Cons

- Training ends up being very unstable to domain shifts (admitted in openreview)
- Limitations themselves are not discussed
- Practical results about representation do not out-perform previous baselines
  The last critic was given by Reviewer 4H5f.
  Is this an issue ?