

Logistics

- Homework 4
 - Due Sunday March 24th (still have two slip days
 - Shorter assignment on VAEs and Diffusion
 - Pinned posts
- Feedback form for HW3 and associated content is due on tomorrow
- Reselased project feedback and HW2 feedback
 - Check graded documents for feedback!
- Midterm next Thursday (03/28)
 - During regular class time
 - \circ $\;$ Alternate time offered Wednesday at (03/27) $\;$
 - \circ $\;$ Location and time will be posted on Ed

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Denoising Diffusion Models

Denoising diffusion models consist of two processes:

- Forward diffusion process that gradually adds noise to input
- Reverse denoising process that learns to generate data by denoising



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Details: Forward Process

Can sample \mathbf{x}_t in closed-form as $q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad \bar{\alpha}_t \in (0, 1)$$









Cornell Bowers CNS Training: Principled Derivation Find the model that maximizes the likelihood of the training data .e. same as VAEs, variational inference; approximate the true posterior









Cornell Bowers CVS Darameterizing the Denoising Model Since both $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ and $p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)$ are Normal distributions, the KL divergence has a simple form: $L_{t-1} = D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)||p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t)) = \mathbb{E}_q \left[\frac{1}{2\sigma_t^2}||\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta}(\mathbf{x}_t, t)||^2\right] + C$ Recall that $\mathbf{x}_t = \sqrt{\alpha_t} \mathbf{x}_0 + \sqrt{(1 - \alpha_t)} \mathbf{\epsilon}$. Ho et al. NeurIPS 2020 observe that: $\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{1}{\sqrt{1 - \beta_t}} \left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1 - \alpha_t}}\mathbf{\epsilon}\right)$ They propose to represent the mean of the denoising model using a *Insise-prediction* network: $\mu_{\theta}(\mathbf{x}_t, t) = \frac{1}{\sqrt{1 - \beta_t}} \left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1 - \alpha_t}} \left[\mathbf{e}(\mathbf{x}_t, t)\right]\right)$ With this parameterization $L_{t-1} = \mathbb{E}_{\mathbf{x}_0 \sim \eta(\mathbf{x}_0), t \sim \mathcal{N}(0, t)} \left[\frac{\beta_t^2}{2\sigma_t^2(1 - \beta_t)(1 - \alpha_t)} ||\mathbf{\epsilon} - \left[\mathbf{e}(\sqrt{\alpha_t} \mathbf{x}_0 + \sqrt{1 - \alpha_t} \mathbf{\epsilon}, t)\right]|^2\right] + C$

http://cs231n.stanford.edu/slides/2023/lecture_15.pdf

Cornel Bowers CIS $\mathbf{x}_{t} = \sqrt{\overline{\alpha}_{t}} \mathbf{x}_{0} + \sqrt{1 - \overline{\alpha}_{t}} \epsilon, \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ Training Objective Weighting ELBO objective leads to a specific regression weight at each time step: $L_{t-1} = \mathbb{E}_{\mathbf{x}_{0} \sim q(\mathbf{x}_{0}), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \underbrace{\left[\underbrace{\frac{\beta_{t}^{2}}{2\sigma_{t}^{2}(1 - \beta_{t})\left[(1 - \overline{\alpha}_{t})\right]}}_{\lambda_{t}} ||\epsilon - \epsilon_{\theta}(\sqrt{\overline{\alpha}_{t}} \mathbf{x}_{0} + \sqrt{1 - \overline{\alpha}_{t}} \epsilon, t)||^{2} \right]}_{\lambda_{t}}$ However, this weight is often very large for small t's Ho et al., 2020 proposed the following objective to improve perceptual quality: $L_{simple} = \mathbb{E}_{\mathbf{x}_{0} \sim q(\mathbf{x}_{0}), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), t \sim \mathcal{U}(1, T)} \left[||\epsilon - \epsilon_{\theta}(\sqrt{\overline{\alpha}_{t}} \mathbf{x}_{0} + \sqrt{1 - \overline{\alpha}_{t}} \epsilon, t)||^{2} \right]$

http://cs231n.stanford.edu/slides/2023/lecture_15.pdf

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People often use U-Nets with residual blocks and self-attention layers at low resolutions

Has same input and output image dimensions



Time representation: sinusoidal positional embeddings

Inject time embedding throughout the network (e.g. additive positional embedding)

tp://cs231n.stanford.edu/slides/2023/lecture_15.pdf

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Diffusion Results

Outperforms prior generative models when using the **simplified** training objective

ELBO objective performs worse!

-	Model	IS	FID
-	Gated PixelCNN [59]	4.60	65.93
	Sparse Transformer [7]		
	PixelIQN [43]	5.29	49.46
	EBM [11]	6.78	38.2
	NCSNv2 [56]		31.75
	NCSN [55]	8.87 ± 0.12	25.32
FLDO	SNGAN [39]	8.22 ± 0.05	21.7
ELBO	SNGAN-DDLS [4]	9.09 ± 0.10	15.42
	StyleGAN2 + ADA (v1) [29]	9.74 ± 0.05	3.26
I = I = I = I = I = I = I = I = I = I =	Ours (L, fixed isotropic Σ)	7.67 ± 0.13	13.51
$L_{\text{simple}} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(0, \mathbf{I}), t \sim \mathcal{U}(1, T)} \left[\epsilon - \epsilon_{\theta} (\underbrace{\sqrt{\alpha_t \ \mathbf{x}_0} + \sqrt{1 - \alpha_t}}_{t \in \tau} \epsilon, t) ^{-} \right]$	Ours (L_{simple})	$9.46 {\pm} 0.11$	3.17
\mathbf{x}_t	Ho et al. 2020		



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Alternative Diffusion Parameterization: Data Prediction

Can also view the diffusion network as learning to predict the original data

$$\mathbf{x}_{t} = \sqrt{\overline{\alpha}_{t}}\mathbf{x}_{0} + \sqrt{1 - \overline{\alpha}_{t}}\epsilon$$
$$\implies \mathbf{x}_{0} = \frac{\mathbf{x}_{t} - \sqrt{1 - \overline{\alpha}_{t}}\epsilon}{\sqrt{\overline{\alpha}_{t}}}$$
$$\implies \mathbf{x}_{\theta}(\mathbf{x}_{t}, t) = \frac{\mathbf{x}_{t} - \sqrt{1 - \overline{\alpha}_{t}}\epsilon_{\theta}(\mathbf{x}_{t}, t)}{\sqrt{\overline{\alpha}_{t}}}$$

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Alternative Diffusion Parameterization: Data Prediction

Can also view the diffusion network as learning to predict the original data

$$\mathbf{x}_{\theta}(\mathbf{x}_t, t) = \frac{\mathbf{x}_t - \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t)}{\sqrt{\bar{\alpha}_t}}$$

Diffusion training objective: $\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)} \left[D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0) \parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)) \right]$

For sampling, want $q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0)$, but don't have access to the original data

Use our estimate of the original data, $\mathbf{x}_{\theta}(\mathbf{x}_t, t)$, to sample:

 $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t) = q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \mathbf{x}_{\boldsymbol{\theta}}(\mathbf{x}_t, t)) \approx q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \mathbf{x}_0)$





Sampling Algorithm











Cornell Bowers CAS Stable Diffusion Demo!

https://huggingface.co/spaces/stabilityai/stable-diffusion

Sample input: "messi as a real madrid player"





Score-based Models

Would like to model the probability density function as follows:

$$p_{ heta}(\mathbf{x}) = rac{e^{-f_{ heta}(\mathbf{x})}}{Z_{ heta}}$$

Discuss: Any problems with directly modelling this?

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Score-based Models

Would like to model the probability density function as follows:

$$p_{ heta}(\mathbf{x}) = rac{e^{-f_{ heta}(\mathbf{x})}}{Z_{ heta}}$$

Want to maximize the log-likelihood of the data:

$$\max_{ heta} \sum_{i=1}^N \log p_ heta(\mathbf{x}_i).$$

Instead approximate the score function:

$$\mathbf{s}_{ heta}(\mathbf{x}) =
abla_{\mathbf{x}} \log p_{ heta}(\mathbf{x}) = -
abla_{\mathbf{x}} f_{ heta}(\mathbf{x}) - \underbrace{
abla_{\mathbf{x}} \log Z_{ heta}}_{=0} = -
abla_{\mathbf{x}} f_{ heta}(\mathbf{x})$$



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Training Objective for noise level t:

$$\sum_{t=1}^T \lambda(t) \mathbb{E}_{\mathbf{x},t} [\|\mathbf{s}_{ heta}(\mathbf{x_t},t) -
abla_{\mathbf{x_t}} \log p_t(\mathbf{x_t})\|_2^2]$$

Using results from denoising score matching [1]:

$$\sum_{t=1}^T \lambda(t) \mathbb{E}_{\mathbf{x},t} [\|\mathbf{s}_{ heta}(\mathbf{ ilde{x}},t) -
abla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t|\mathbf{x})\|_2^2]$$

Using the definition of the pdf of a gaussian,

$$\sum_{t=1}^T \lambda(t) \mathbb{E}_{\mathbf{x},t} [\|\mathbf{s}_{ heta}(\mathbf{x}_t,t) - rac{\mathbf{x}_t - \mathbf{x}}{\sigma_t^2}\|_2^2]$$

[1] P. Vincent. A connection between score matching and denoising autoencoders. Neural computation, 23(7):1661–1674, 2011.

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 $\mathbf{x_t} \sim \mathcal{N}(\mathbf{x}, \sigma_t^2 I)$

Discuss: How does this training objective relate to that of DDPMs?

$$\sum_{t=1}^T \lambda(t) \mathbb{E}_{\mathbf{x},t}[\|\mathbf{s}_ heta(\mathbf{x}_t,t) - rac{\mathbf{x}_t - \mathbf{x}}{\sigma_t^2}\|_2^2]$$

Continuous time (Stochastic Differential Equation Perspective)



Continuous time (Stochastic Differential Equation Perspective) $\overrightarrow{P} = e^{-\frac{1}{2}} e^{-\frac{1}{2$

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Conditional Diffusion

- We want to condition on images or text
- Learn a conditional diffusion model



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Conditional Diffusion with Classifier Guidance

- May not have access to paired data for training
- Use Bayes' rule to decompose the conditional score into the unconditional score and a likelihood term

$$abla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t|\mathbf{y}) =
abla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t) +
abla_{\mathbf{x}_t} \log p_t(\mathbf{y}|\mathbf{x}_t)$$

Only need to train a classifier on noised data



Dhariwal, P., & Nichol, A. (2021). Diffusion models beat gans on image synthesis. Advances in neural information processing systems, 34, 8780-8794.

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Classifier-Free Guidance

- Train a joint conditional and unconditional diffusion model
- Conditioning information is added by concatenating to input or cross attending
- Modified conditional distribution

 $\log { ilde p}_t(\mathbf{x}_t|\mathbf{y}) \propto \ p_t(\mathbf{x}_t|\mathbf{y}) \ p_t(\mathbf{y}|\mathbf{x}_t)^w$

Conditional sampling

$$abla_{\mathbf{x}_t} \log ilde{p}_t(\mathbf{x}_t | \mathbf{y}) =
abla_{\mathbf{x}_t} \log \, p_t(\mathbf{x}_t) + w(
abla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t | \mathbf{y}) -
abla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t))$$

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Classifier-Free Guidiance

Significantly improves quality of conditional models

Used by practically **every** conditional diffusion model

Increasing Guidance

Saharia, C., Chan, W., Saxena, S., Li, L., Whang, J., Denton, E. L., ... & Norouzi, M. (2022). Photorealistic text-to-image diffusion models with deep language understanding. Advances in neural information processing systems. 35, 36479-36494







High-Resolution Image Synthesis with Latent Diffusion Models



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Impact of Patch Discriminator







Reconstruction with Discriminator

Discriminator https://neurips2023-ldm-tutorial.github.io/



Latent Diffusion

Many state-of-the-art large-scale text-to-image models are latent diffusion models

- Stability Al's Stable Diffusion
- Meta's Emu
- OpenAl's Dall-E 3







Prompt: 3D animation of a small, round, fluffy creature with big, expressive eyes explores a vibrant, enchanted forest.

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vibrant, enchanted forest.

Prompt: 3D animation of a small, round, fluffy creature with big, expressive eyes explores a



Prompt: A cat waking up its sleeping owner demanding breakfast.

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Review

- Diffusion models can be used to generate high quality samples
- They were introduced simultaneously from two different perspecteives
- Conditional diffusion models can be used to generate samples conditioned on other text or image
- Diffusion can also be performed in latent spaces