Combining Generative Model Families

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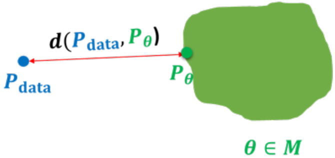
Lecture 15

Announcements

- Assignment 3 is due next Monday
- Please review your project proposal feedback. Project progress report due on 3/31.

Recap So Far

$\mathbf{x}_i \sim P_{\text{data}}$
$i = 1, 2, \ldots, n$



Model family

We have seen several generative models and several tasks:

1. **Generation**: Autoregressive, Latent Variable Models, GANs, Score-Based & Diffusion Models
2. **Density Estimation and Outlier Detection**: Autoregressive Models, Normalizing Flows, Energy-Based Models
3. **Representation Learning**: Latent Variable Models

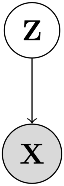
Can we combine generative models to do even better on certain tasks?

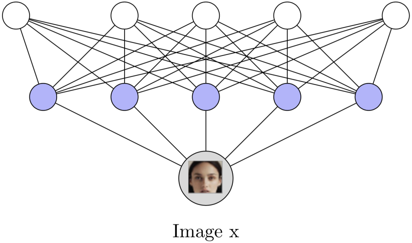
Lecture Outline

1. Combining Model Families
    - Autoregressive models + VAEs: PixelVAE
    - Autoregressive models + Flows: Autoregressive flows
    - Flows + VAEs: Flow-based posteriors
    - VAEs + RNNs: Variational RNNs
    - Flows + GANs: FlowGAN
    - GANs + VAEs: InfoGAN, InfoVAE, β-VAE

Recall: Deep Gaussian Latent Variable Models (VAEs)

We may form deep latent variable models by parameterizing the $\mathbf{z} \rightarrow \mathbf{x}$ mapping using neural nets. Deep Gaussian models are an example:



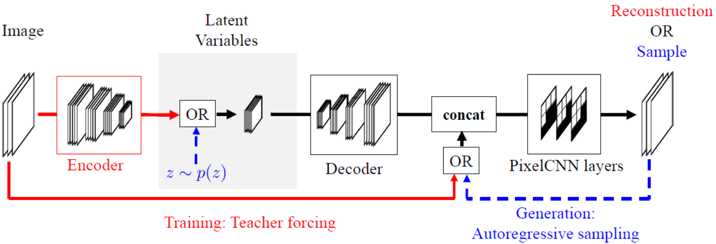


1. The prior $p(\mathbf{z})$ is a p-dimensional Gaussian $\mathcal{N}(0, I_p)$
2. $p(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mu_\theta(\mathbf{z}), \Sigma_\theta(\mathbf{z}))$ where μ_θ,Σ_θ are neural networks

The $\mathbf{z}$ form a smooth parameterization of faces $\mathbf{x}$.

PixelVAE (Gulrajani et al., 2017)

The PixelVAE model combines autoregressive PixelCNNs and VAEs:



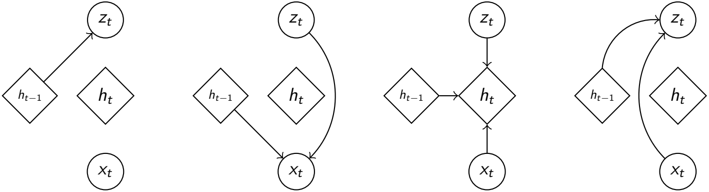
Gulrajani et. al, 2017

- $\mathbf{z}$ is transformed into a feature map with the same resolution as $\mathbf{x}$
- Autoregressive structure: $p(\mathbf{x} \mid \mathbf{z}) = \prod_i p(x_i \mid x_1, \cdots, x_{i-1}, \mathbf{z})$
  - $p(\mathbf{x} \mid \mathbf{z})$ is a PixelCNN
  - Prior $p(\mathbf{z})$ can also be autoregressive
- State-of-the art log-likelihood on some datasets; learns features (unlike PixelCNN); computationally cheaper than PixelCNN (shallower)

Variational RNN (Chung et al., 2015)

- **Goal:** Learn a joint distribution over a sequence $p(x_1, \cdots, x_T)$
- Use VAE for sequential data, using latent variables $z_1, \cdots, z_T$ (one/step)

$$p(x_{\leq T}, z_{\leq T}) = \prod_{t=1}^{T} p(x_t \mid z_{\leq t}, x_{<t}) p(z_t \mid z_{<t}, x_{<t})$$



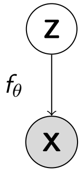
(a) Prior (b) Generation (c) Recurrence (d) Inference

Chung et al, 2016

- Use RNNs to model the conditionals (similar to PixelRNN)
- Use RNNs for inference $q(z_{\leq T} | x_{\leq T}) = \prod_{t=1}^{T} q(z_t \mid z_{<t}, x_{\leq t})$
- Train like VAE to maximize ELBO. Conceptually similar to PixelVAE.

Recall: Autoregressive Flows

Flows and autoregressive models are also closely related.



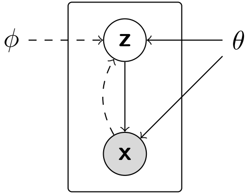
- Flow model, the marginal likelihood $p(\mathbf{x})$ is given by

$$p_X(\mathbf{x};\theta) = p_Z\left(\mathbf{f}_\theta^{-1}(\mathbf{x})\right)\left|\det\left(\frac{\partial \mathbf{f}_\theta^{-1}(\mathbf{x})}{\partial \mathbf{x}}\right)\right|$$

  where $p_Z(\mathbf{z})$ is usually simple (e.g., Gaussian). More complex prior?
- Prior $p_Z(\mathbf{z})$ can be autoregressive $p_Z(\mathbf{z}) = \prod_i p(z_i \mid z_1, \cdots, z_{i-1})$.
- Autoregressive models are related to flows. Just another MAF layer.
- Autoregressive flow models can be naturally stacked.

VAE + Flow Model (Kingma et al., 2016)

Flows can improve the expressivity of variational posteriors in VAEs.



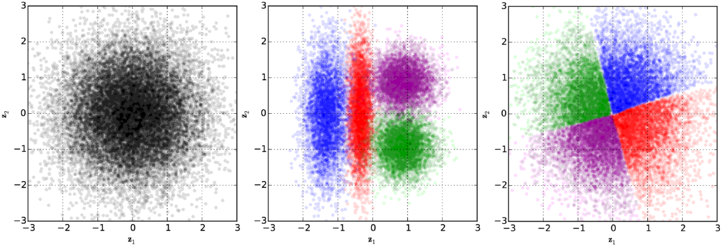
$$\log p(\mathbf{x};\theta) \geq \sum_{\mathbf{z}} q(\mathbf{z}|\mathbf{x};\phi)\log p(\mathbf{z},\mathbf{x};\theta) + H(q(\mathbf{z}|\mathbf{x};\phi)) = \underbrace{\mathcal{L}(\mathbf{x};\theta,\phi)}_{\text{ELBO}}$$

$$\log p(\mathbf{x};\theta) = \mathcal{L}(\mathbf{x};\theta,\phi) + \underbrace{D_{KL}(q(\mathbf{z}\mid\mathbf{x};\phi)\|p(\mathbf{z}|\mathbf{x};\theta))}_{\text{Gap between true log-likelihood and ELBO}}$$

- $q(\mathbf{z}|\mathbf{x};\phi)$ is often too simple (Gaussian) compared to the true posterior $p(\mathbf{z}|\mathbf{x};\theta)$, hence ELBO bound is loose
- **Idea:** Make posterior more flexible: $\mathbf{z}' \sim q(\mathbf{z}'|\mathbf{x};\phi)$, $\mathbf{z} = f_{\phi'}(\mathbf{z}')$ for an invertible $f_{\phi'}$ (Rezende and Mohamed, 2015; Kingma et al., 2016)
- Still easy to sample from, and can evaluate density.

VAE + Flow Model (Kingma et al., 2016)

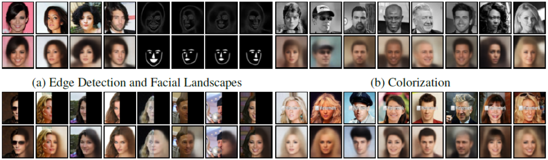
Consider a dataset with four datapoints, shown in different colors below.



(a) Prior distribution (b) Posteriors in standard VAE (c) Posteriors in VAE with IAF

- The VAE has a Gaussian prior (left figure).
- The approximate posterior $q(\mathbf{z}|\mathbf{x})$ is also Gaussian. Hence each colored "cloud" of samples for each datapoint $\mathbf{x}$ is also Gaussian (middle).
- Flows make $q(\mathbf{z}|\mathbf{x})$ non-Gaussian. Hence, they fit the prior better.
- Posterior approximation is more flexible, hence we can get tighter ELBO (closer to true log-likelihood).

Often, data features different modalities ("views"); we may fit these jointly.

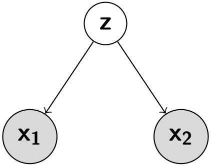


(a) Edge Detection and Facial Landscapes (b) Colorization

(c) Fill in the Blank (d) Removing Watermarks

Wu and Goodman, 2018

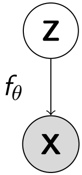
- **Goal:** Learn a joint distribution over the two domains $p(x_1, x_2)$, e.g., color and gray-scale images Can use a VAE style model:



- Learn $p_\theta(x_1, x_2)$, use inference nets $q_\phi(z \mid x_1)$, $q_\phi(z \mid x_2)$, $q_\phi(z \mid x_1, x_2)$.

Combining Losses

Consider a standard flow model $\mathbf{x} = f_\theta(\mathbf{z})$.

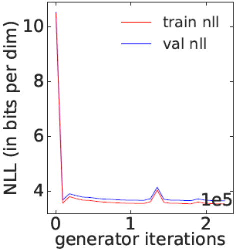


- The marginal likelihood $p(\mathbf{x})$ is given by

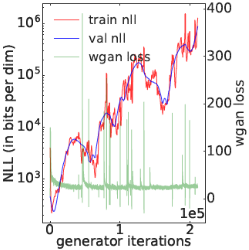
$$p_X(\mathbf{x};\theta) = p_Z\left(\mathbf{f}_\theta^{-1}(\mathbf{x})\right)\left|\det\left(\frac{\partial \mathbf{f}_\theta^{-1}(\mathbf{x})}{\partial \mathbf{x}}\right)\right|.$$

- Can also be thought of as the generator of a GAN
- Should we train by $\min_\theta D_{KL}(p_{data}, p_\theta)$ or $\min_\theta JSD(p_{data}, p_\theta)$?

FlowGAN (Grover et al., 2018)



(a) MLE



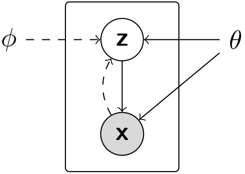
(b) ADV

Although $D_{KL}(p_{data}, p_\theta) = 0$ if and only if $JSD(p_{data}, p_\theta) = 0$, optimizing one does not necessarily optimize the other. If $\mathbf{z}, \mathbf{x}$ have same dimensions, can optimize $\min_\theta KL(p_{data}, p_\theta) + \lambda JSD(p_{data}, p_\theta)$

Objective	Inception Score	Test NLL (in bits/dim)
MLE	2.92	**3.54**
ADV	**5.76**	8.53
Hybrid ($\lambda = 1$)	3.90	4.21

Interpolates between a GAN and a flow model

Combining VAEs + GANs



$$\log p(\mathbf{x};\theta) = \underbrace{\mathcal{L}(\mathbf{x};\theta,\phi)}_{\text{ELBO}} + D_{KL}(q(\mathbf{z} \mid \mathbf{x};\phi) \| p(\mathbf{z}|\mathbf{x};\theta))$$

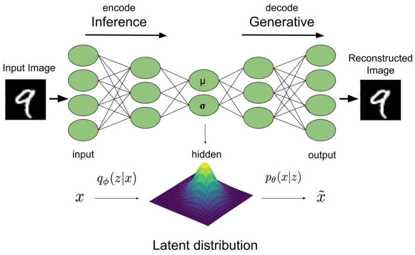
$$\underbrace{E_{\mathbf{x}\sim p_{data}}[\mathcal{L}(\mathbf{x};\theta,\phi)]}_{\approx\text{training obj.}} = E_{\mathbf{x}\sim p_{data}}\left[\log p(\mathbf{x};\theta) - D_{KL}(q(\mathbf{z} \mid \mathbf{x};\phi) \| p(\mathbf{z}|\mathbf{x};\theta))\right]$$

$$\overset{\text{up to const.}}{\equiv} -\underbrace{D_{KL}(p_{data}(\mathbf{x}) \| p(\mathbf{x};\theta))}_{\text{equiv. to MLE}} - E_{\mathbf{x}\sim p_{data}}\left[D_{KL}(q(\mathbf{z} \mid \mathbf{x};\phi) \| p(\mathbf{z}|\mathbf{x};\theta))\right]$$

- Note: regularized maximum likelihood estimation (Shu et al, *Amortized inference regularization*)
- Can add in a GAN objective $-JSD(p_{data}, p(\mathbf{x};\theta))$ to get sharper samples, i.e., discriminator attempting to distinguish VAE samples from real ones.

Adversarial Autoencoders

Recall the autoencoder perspective on VAEs:



- VAE are latent models $p_\theta(\mathbf{x}) = \int p_\theta(\mathbf{x}, \mathbf{z}) d\mathbf{z}$ that optimize the ELBO

$$\mathcal{L}(\mathbf{x}; \theta, \phi) = E_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p(\mathbf{x}|\mathbf{z}; \theta)] - D_{KL}(q_\phi(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))$$

- We may also match features using the JSD instead of the KLD. Matching $p(z)$ and $q_\phi(\mathbf{z}|\mathbf{x})$ is done in a GAN-style manner.

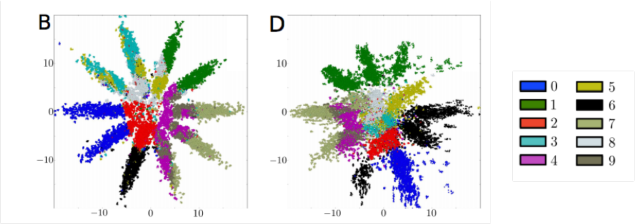
$$\mathcal{L}(\mathbf{x}; \theta, \phi) = E_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p(\mathbf{x}|\mathbf{z}; \theta)] - D_{JSD}(q_\phi(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))$$

- This yields adversarial auto-encoders.

Adversarial Autoencoders (Makhazani et al., 2018)

Adversarial autoencoders can produce better match the latent priors.

- In this example, the prior is a mixture of 10 Gaussians. Left figure shows an AAE posterior; right figure shows a VAE posterior.



Source: Makhzani et al., 2018

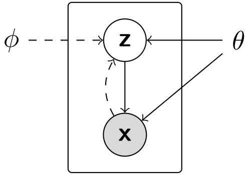
- Adversarial autoencoders don't need to assume $q(z|x)$ is Gaussian
- They can also better match the true shape of the prior (imagine it being an image).

A Reformulation of the ELBO

Next, consider the following reformulation of the ELBO:

$$
\begin{aligned}
\underbrace{E_{\mathbf{x}\sim p_{data}}[\mathcal{L}(\mathbf{x};\theta,\phi)]}_{\approx\text{training obj.}} \quad &= \quad E_{\mathbf{x}\sim p_{data}}\left[\log p(\mathbf{x};\theta) - D_{KL}(q(\mathbf{z}\mid\mathbf{x};\phi)\|p(\mathbf{z}|\mathbf{x};\theta))\right] \\
&\overset{\text{up to const.}}{\equiv} -D_{KL}(p_{data}(\mathbf{x})\|p(\mathbf{x};\theta)) - E_{\mathbf{x}\sim p_{data}}\left[D_{KL}(q(\mathbf{z}\mid\mathbf{x};\phi)\|p(\mathbf{z}|\mathbf{x};\theta))\right] \\
&= \quad -\sum_{\mathbf{x}} p_{data}(\mathbf{x})\left(\log\frac{p_{data}(\mathbf{x})}{p(\mathbf{x};\theta)} + \sum_{\mathbf{z}} q(\mathbf{z}\mid\mathbf{x};\phi)\log\frac{q(\mathbf{z}\mid\mathbf{x};\phi)}{p(\mathbf{z}|\mathbf{x};\theta)}\right) \\
&= \quad -\sum_{\mathbf{x}} p_{data}(\mathbf{x})\left(\sum_{\mathbf{z}} q(\mathbf{z}\mid\mathbf{x};\phi)\log\frac{q(\mathbf{z}\mid\mathbf{x};\phi)p_{data}(\mathbf{x})}{p(\mathbf{z}|\mathbf{x};\theta)p(\mathbf{x};\theta)}\right) \\
&= \quad -\sum_{\mathbf{x},\mathbf{z}} p_{data}(\mathbf{x})q(\mathbf{z}\mid\mathbf{x};\phi)\log\frac{p_{data}(\mathbf{x})q(\mathbf{z}\mid\mathbf{x};\phi)}{p(\mathbf{x};\theta)p(\mathbf{z}|\mathbf{x};\theta)} \\
&= \quad -D_{KL}(\underbrace{p_{data}(\mathbf{x})q(\mathbf{z}\mid\mathbf{x};\phi)}_{q(\mathbf{z},\mathbf{x};\phi)}\,\|\,\underbrace{p(\mathbf{x};\theta)p(\mathbf{z}|\mathbf{x};\theta)}_{p(\mathbf{z},\mathbf{x};\theta)})
\end{aligned}
$$

Ignoring Latent Variables: A VAE Failure Mode



$$E_{\mathbf{x}\sim p_{data}}[\underbrace{\mathcal{L}(\mathbf{x};\theta,\phi)}_{\text{ELBO}}] \equiv -D_{KL}(\underbrace{p_{data}(\mathbf{x})q(\mathbf{z}\mid\mathbf{x};\phi)}_{q(\mathbf{z},\mathbf{x};\phi)} \,\|\, \underbrace{p(\mathbf{x};\theta)p(\mathbf{z}|\mathbf{x};\theta)}_{p(\mathbf{z},\mathbf{x};\theta)})$$

- ELBO is optimized as long as $q(\mathbf{z},\mathbf{x};\phi) = p(\mathbf{z},\mathbf{x};\theta)$. Many solutions are possible! For example,
  1. $p(\mathbf{z},\mathbf{x};\theta) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z};\theta) = p(\mathbf{z})p_{data}(\mathbf{x})$
  2. $q(\mathbf{z},\mathbf{x};\phi) = p_{data}(\mathbf{x})q(\mathbf{z}|\mathbf{x};\phi) = p_{data}(\mathbf{x})p(\mathbf{z})$
  3. Note: $\mathbf{x}$ and $\mathbf{z}$ are independent. $\mathbf{z}$ carries no information about $\mathbf{x}$. This happens in practice when $p(\mathbf{x}|\mathbf{z};\theta)$ is too flexible, like PixelCNN.
- **Issue:** Many more variables than constraints

InfoVAE and InfoGAN

- Explicitly add a mutual information term to the objective

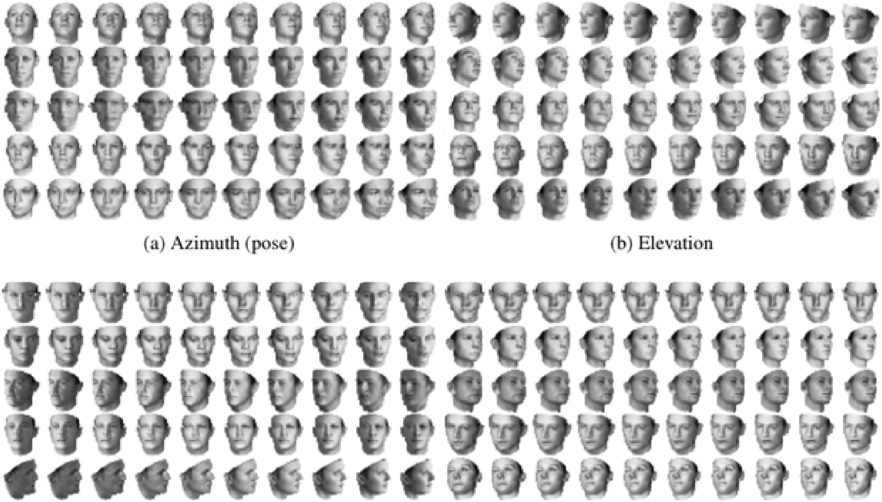
$$-D_{KL}(\underbrace{p_{data}(\mathbf{x})q(\mathbf{z} \mid \mathbf{x};\phi)}_{q(\mathbf{z},\mathbf{x};\phi)} \,\|\, \underbrace{p(\mathbf{x};\theta)p(\mathbf{z}|\mathbf{x};\theta)}_{p(\mathbf{z},\mathbf{x};\theta)}) + \alpha MI(\mathbf{x},\mathbf{z})$$

- MI intuitively measures how far **x** and **z** are from being independent

$$MI(\mathbf{x},\mathbf{z}) = D_{KL}\left(p(\mathbf{z},\mathbf{x};\theta) \| p(\mathbf{z})p(\mathbf{x};\theta)\right)$$

- InfoGAN (Chen et al, 2016) use mutual information to learn meaningful (disentangled) representations of the data

InfoGAN



(a) Azimuth (pose) (b) Elevation

(c) Lighting (d) Wide or Narrow

β-VAE

Model proposed to learn disentangled features (Higgins, 2016)

$$-E_{q_\phi(\mathbf{x},\mathbf{z})}[\log p_\theta(\mathbf{x}|\mathbf{z})] + \beta E_{\mathbf{x}\sim p_{data}} [D_{KL}(q_\phi(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}))]$$

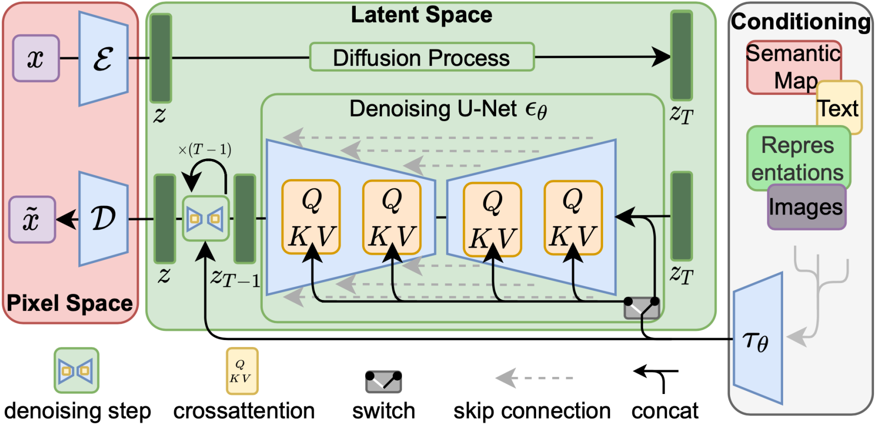
It is a VAE with scaled up KL divergence term. This is equivalent (up to constants) to the following objective:

$$(\beta - 1)MI(\mathbf{x};\mathbf{z}) + \beta D_{KL}(q_\phi(\mathbf{z})\|p(\mathbf{z})) + E_{q_\phi(\mathbf{z})}[D_{KL}(q_\phi(\mathbf{x}|\mathbf{z})\|p_\theta(\mathbf{x}|\mathbf{z}))]$$

See *The Information Autoencoding Family: A Lagrangian Perspective on Latent Variable Generative Models* for more examples.

Latent Diffusion: VAE + Diffusion (Rombach et al., 2022)

Diffusion can be run in the latent space of a VAE for increased efficiency.



Latent Diffusion: VAE + Diffusion (Rombach et al., 2022)

"[...] steampunk flying machine in the sky with cogs and mechanisms [...]"

More Extensions of Diffusion Models

- Adversarial Score Matching (Jolicoeur-Martineau et al. 2021): Diffusion + GANs.
  - Diffusion models can be also seen as producing denoised $\hat{\mathbf{x}}_0(\mathbf{x}_t)$.
  - Fit $\hat{\mathbf{x}}_0(\mathbf{x}_t) \approx x_0$ using an adversarial loss (JSD).
- Autoregressive Diffusion Models (Hoogeboom at al. 2021)
  - Autoregressive process can be seen as undoing deletion-based noising.
  - ARDMs can undo this noising process following any order.

Conclusion

- We have covered several useful building blocks: autoregressive, latent variable models, flow models, GANs.
- Can be combined in many ways to achieve different tradeoffs: many of the models we have seen today were published in top ML conferences in the last couple of years
- Lots of room for exploring alternatives in your projects!
- Which one is best? Evaluation is tricky. Still largely empirical