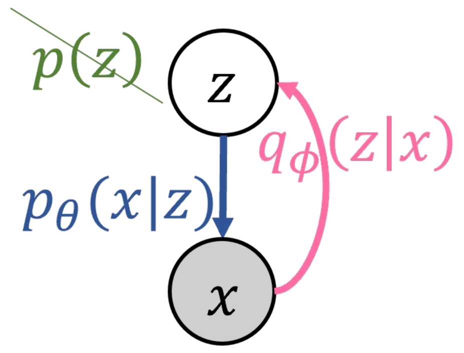

On the Generative Utility of Cyclic Conditionals

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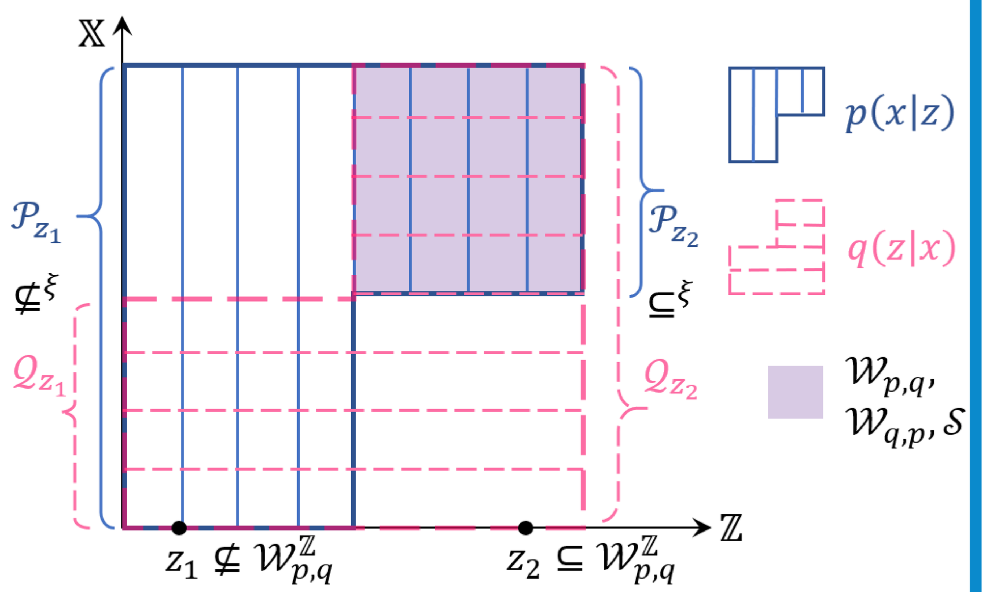
The Question

Can we determine a **joint** distribution $p(x,z)$ only using two **conditional** distributions $p(x|z)$ and $q(z|x)$ that form a cycle?

- **Compatibility**: is there a common joint that induces both conditionals?
- **Determinacy**: is the common joint unique?

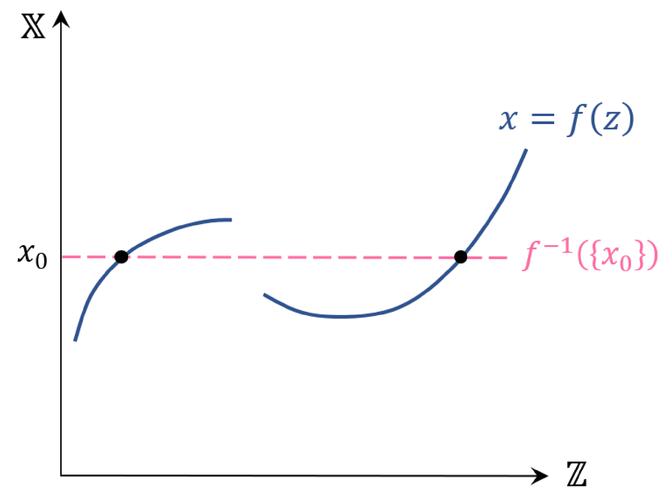
The Answer: Theory

Absolutely-Continuous Case:
"smooth" distr. on continuous spaces, all distr. on discrete spaces.



- VAE, diffusion-based.
- **Thm**: **Compatibility** is achieved, iff on a suitable set $\mathcal{S} \subseteq \mathbb{X}\times\mathbb{Z}$ constructed from the conditional densities, $\frac{p(x|z)}{q(z|x)}$ a.e. **factorizes** as $a(x)b(z)$, where $a(x)$ is integrable.
  - Equivalence condition, operable, self-contained.
  - Why complicated: conditionals can be arbitrary on a set of marginal measure zero (*e.g.*, outside the marginal support).
- **Thm**: **Determinacy** is achieved on $\mathcal{S}$, if $\mathcal{S}$ is "rectangular": $\mathcal{S}_z \overset{\text{a.s.}}{=} \mathcal{S}^{\mathbb{X}}, \forall$ a.e. $z \in \mathcal{S}^{\mathbb{Z}}$ and $\mathcal{S}_x \overset{\text{a.s.}}{=} \mathcal{S}^{\mathbb{Z}}, \forall$ a.e. $x \in \mathcal{S}^{\mathbb{X}}$.
  - Determinacy is only possible on each $\mathcal{S}$.
  - If both densities have *full support*, $\mathbb{X}\times\mathbb{Z}$ is the only $\mathcal{S}$.

Dirac Case:
$p(\mathcal{X}|z) = \delta_{f(z)}(\mathcal{X}) := \mathbb{I}[f(z) \in \mathcal{X}]$.



- Incl. BiGAN, flow-based.
- **Thm**: **Compatibility** is achieved, iff $\exists x_0$ s.t. $q(f^{-1}(\{x_0\})|x_0) = 1$: q puts mass only on the pre-image.
  - Only one x_0 suffices: $\delta_{(x_0, f(x_0))}$ is a common joint.
  - When $q(\mathcal{Z}|x) = \delta_{g(x)}(\mathcal{Z})$, min. **cycle-consistency loss** $\mathbb{E}_{p_{\text{ref}}(x)}\ell(x, f(g(x)))$ is sufficient.
  - Flow-based models are natually compatible.
- **Determinacy**:
  - On each $\{x_0\}$, the joint $\delta_{(x_0,f(x_0))}$ is unique.
  - If such x_0 is not unique, the joint is not unique on $\mathbb{X}\times\mathbb{Z}$: compatible p, q only determine a curve in $\mathbb{X}\times\mathbb{Z}$ but not a distribution on it.

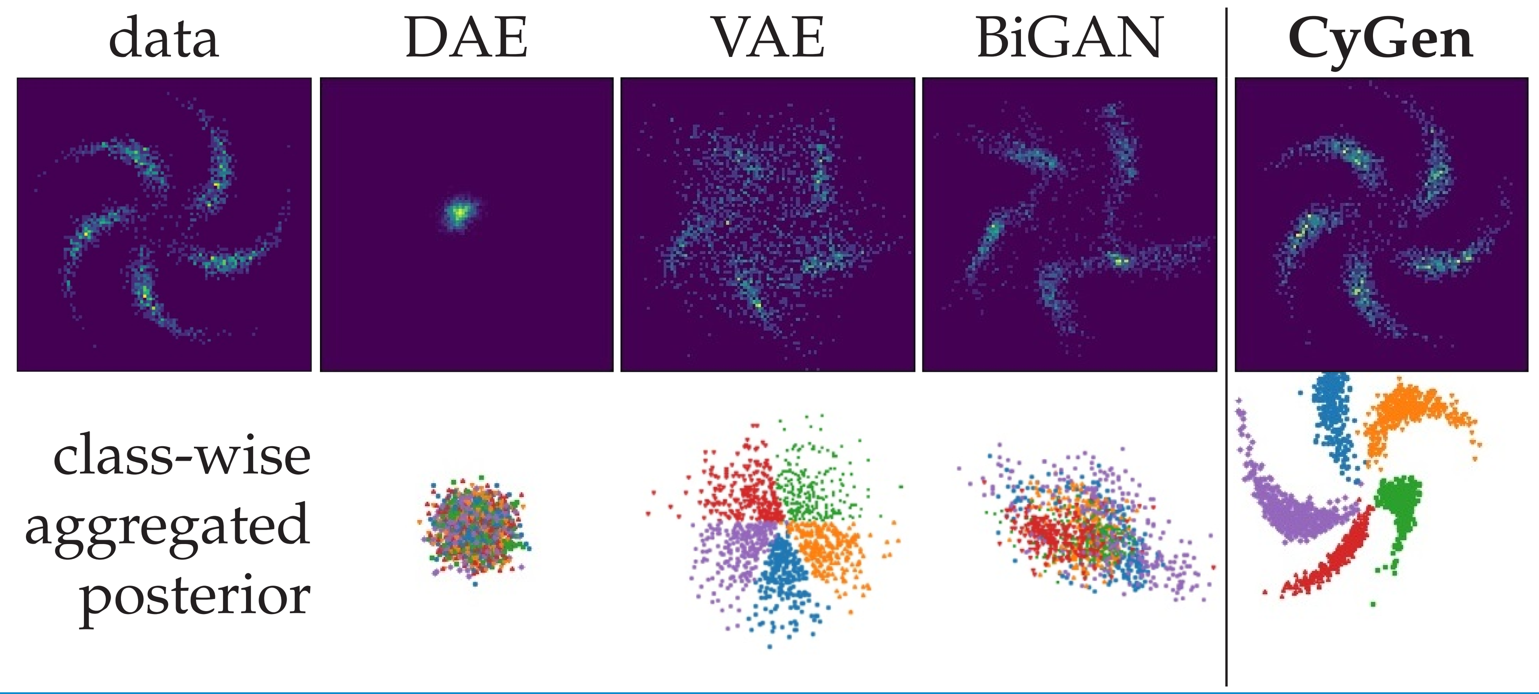
Problems of Current Generative Models

VAE, (Bi)GAN, flow/diffusion-based:

- Need $p(x|z)$ for generation, $q(z|x)$ for representation.
- Use a prior $p(z)$ to define joint $p(x,z) = p(z)p(x|z)$.

Specifying a prior leads to:

- **Manifold mismatch** (hinders generation): the modeled $p(x)$ is restricted to a simply-connected support.
- **Posterior collapse** (hinders representation): representations of different x are squeezed together.

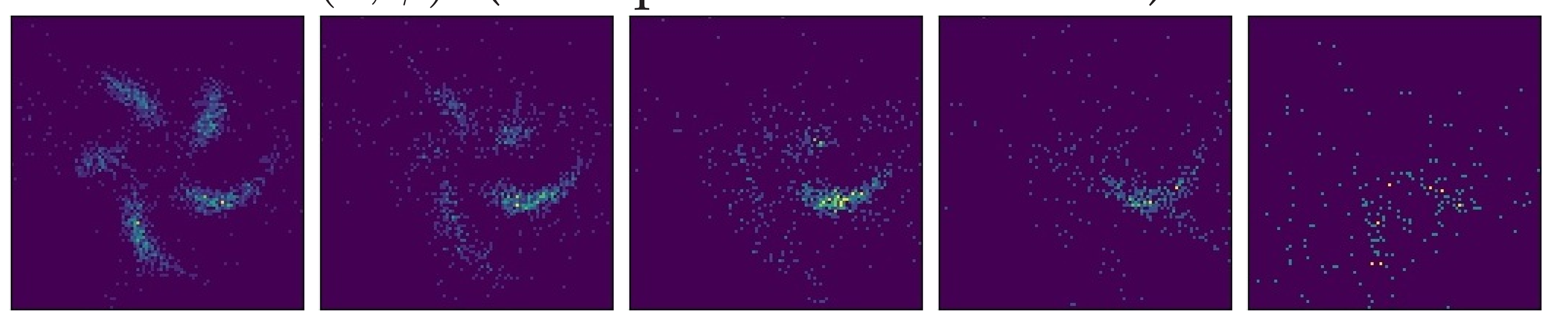


The New Framework: Cyclic-Conditional Generative Model (CyGen)

Eligibility as a generative model:

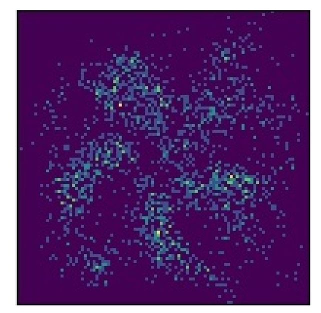
- **Determinacy**: Use absolutely-continuous conditionals, modeled by *fully-supported* densities $p_\theta(x|z)$, $q_\phi(z|x)$ (like VAE).
- **Compatibility**:
  $(\min_{\theta,\phi})\ C(\theta,\phi) := \mathbb{E}_{p_{\text{ref}}(x,z)} \left\| \nabla_x \nabla_z^\top \log\left(p_\theta(x|z)/q_\phi(z|x)\right)\right\|_F^2$.
  - $C(\theta,\phi) = 0 \iff p_\theta(x|z)/q_\phi(z|x)$ a.e. factorizes.
  - Generalizes cycle-consistency loss to *probabilistic* conditionals.
  - Gaussian VAE: $C(\theta,\phi) = 0 \iff$ mean fun. of p, q are affine! For nonlinear repr., one conditional must not be Gaussian.
  - **Scalable** unbiased stochastic estimate: $\mathbb{E}_{p_{\text{ref}}}\mathbb{E}_{p(\eta):\mathbb{E}[\eta]=0,\text{Cov}[\eta]=I} \left\|\nabla_z\left(\eta^\top \nabla_x \log\left(p_\theta(x|z)/q_\phi(z|x)\right)\right)\right\|_2^2$. Reduce $O(d_{\mathbb{X}} d_{\mathbb{Z}})$ to $O(d_{\mathbb{X}} + d_{\mathbb{Z}})$.

In absence of $C(\theta,\phi)$: (after pretrained as a VAE)



Usage as a generative model:

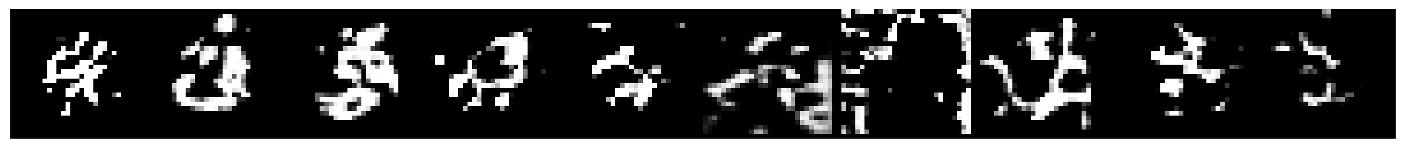
- **Fit data**: max. likelihood est.
  $\log p_{\theta,\phi}(x) = -\log \mathbb{E}_{q_\phi(z'|x)}[1/p_\theta(x|z')]$.
  - Est. expect. by reparameterization and `logsumexp`.
  - Denoising auto-encoder (DAE) objective $\mathbb{E}_{q_\phi(z'|x)}[\log p_\theta(x|z')]$ is improper: **(1)** $\geqslant \log p_{\theta,\phi}(x)$; **(2)** mode-collapses q thus hurts determinacy.
- **Generate data**: dynamics-based MCMC.
  - More efficient than Gibbs sampling: 👉



  - Only requires unnormalized density: $p_{\theta,\phi}(x) \propto \frac{p_\theta(x|z)}{q_\phi(z|x)}, \forall z$.
  - E.g., Stochastic Gradient Langevin Dynamics: $x^{(t+1)} = x^{(t)} + \varepsilon \nabla_{x^{(t)}} \log \frac{p_\theta(x^{(t)}|z^{(t)})}{q_\phi(z^{(t)}|x^{(t)})} + \sqrt{2\varepsilon}\,\eta^{(t)}$, where $z^{(t)} \sim q_\phi(z|x^{(t)})$, $\eta^{(t)} \sim \mathcal{N}(0, I)$.

Real-World Experiments

Data generation and **classification accuracy (%) using representation**:

	MNIST samples	Acc.	SVHN samples	Acc.
DAE		98.0±0.1		74.5±1.0
VAE		94.5±0.3		30.8±0.2
CyGen		**98.3**±0.1		**75.8**±0.5