On the Generative Utility of Cyclic Conditionals

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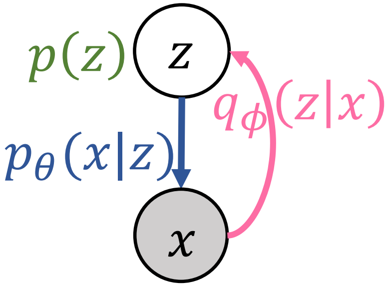
Introduction

The problem:
Whether or when can we model a *joint* distribution $p(x, z)$
only using two *conditional* models $p(x|z)$ and $q(z|x)$ that form a cycle?

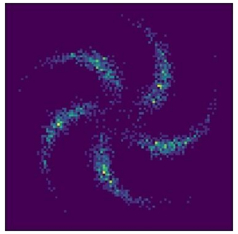
VAE, BiGAN,
flow-based,
diffusion-based



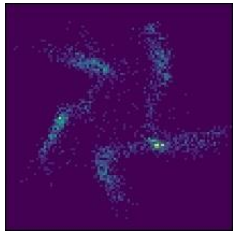
- Motivation from deep generative models:

  Model both $p(x|z)$ for *generation*, and $q(z|x)$ for *representation*.
  Define their common joint by a prior $p(z)$: $p(x, z) \coloneqq p(z)p(x|z)$.
  - Problems of Gaussian prior:
    - **Manifold mismatch**: $p(x)$ has a *simply connected support* as $p(z)$
      $\Longrightarrow$ restricted expressiveness.
    - **Posterior collapse**: $q(z|x)$ is squeezed to the origin
      $\Longrightarrow$ degraded representativeness.

BiGAN repr.



true data distr.



BiGAN data distr.

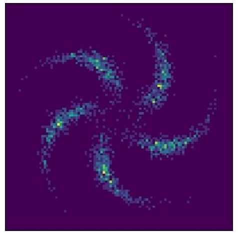
  - Using an informative prior:

    Domain knowledge on the prior is even more scarce than on the conditional models.
    (e.g., shift/rotation invariance of $q(z|x)$ for image representation (CNN/SphereNet))
  - Learning a prior model: additional modeling and training cost.

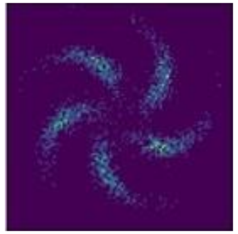
Introduction

The problem:
Whether or when can we model a *joint* distribution $p(x, z)$
only using two *conditional* models $p(x|z)$ and $q(z|x)$ that form a cycle?

- Key sub-problems:
  - **Compatibility** (existence): When the two conditionals can be induced from a common joint.
  - **Determinacy** (uniqueness): When the two *compatible* conditionals uniquely determine a joint.
- In this work,
  - Theory: **compatibility** criteria (equivalent conditions) and sufficient conditions for **determinacy**.
    - Operable and self-contained.
    - Unify continuous and discrete cases.
  - **CyGen**: **Cy**clic-conditional **Gen**erative model.
    - Methods for enforcing compatibility and determinacy, fitting data, and data generation.



true data distr.



CyGen data distr.

CyGen repr.

Related Work: Modeling

- Cyclic conditional models
  - **Dependency networks** [Heckerman'00]:
    No latent variable (so compatibility is not a problem). Gibbs sampling for the joint.
  - **Denoising auto-encoders (DAEs)** [Vincent'08]: $\min \mathbb{E}_{p^*(x) q(z|x)}[\log p(x|z)]$.
    - Variants: Uncertainty AE [Grover'19], Walkback [Bengio'13], GibbsNet [Lamb'17].
    - The loss is not suitable for optimizing $q(z|x)$ (mode-collapse, weakens determinacy).
    - Inefficient generation and unstable training by Gibbs sampling.
  - **Dual learning** [He'16; Xia'17a,b; Lin'19], Disco[Kim'17]/Cycle[Zhu'17]/Dual[Yi'17]-GAN:
    - Not for generative modeling (in fact, they lack determinacy).
    - No latent variable, unpaired data.

Related Work: Theory

- **Compatibility**
  - The classical condition [Arnold’89,01,12] is not necessary.
  - The equivalent condition [Berti’14] is still existential.
  - Results from DAE [Bengio’13,14; Lamb’17; Grover’19]: not self-contained ($p^*(x)$ is required).
  - Cycle-consistency loss [Kim’17; Zhu’17; Yi’17; Lin’19]: only for Dirac (deterministic) conditionals.
- **Determinacy**
  - Determining $p(x)$ through score matching (SM):
    DAE $\Longleftrightarrow$ denoising SM (Gaussian RBM) [Vincent’11].
    DAE $\Longleftrightarrow$ SM (Gaussian decoder noise and infinitesimal Gaussian corruption) [Alain'14].
  - Determining $p(x, z)$ through Gibbs chain:
    - The chain is ergodic thus has a unique stationary distr. $\pi(x, z)$ under a global [Bengio’13; Lamb’17; Grover’19] or local [Bengio’13] shared support condition.
    - When incompatible, $\pi(z|x) \neq q(z|x)$ or $\pi(x|z) \neq p(x|z)$ [Heckerman’00, Bengio’13].
    - No explicit expression. Slow convergence for generation. Unstable training (Walkback, GibbsNet).
  - The classical description [Arnold’12]: restricted to product support; Dirac case not covered.

Theory

Setup

- Measure spaces for random variables x and z: $(\mathbb{X}, \mathscr{X}, \xi)$ and $(\mathbb{Z}, \mathscr{Z}, \zeta)$.
- Product measure space $(\mathbb{X} \times \mathbb{Z}, \mathscr{X} \otimes \mathscr{Z}, \xi \otimes \zeta)$.
- For $\mathcal{W} \in \mathscr{X} \otimes \mathscr{Z}$, define
  its *slice* at z: $\mathcal{W}_z := \{x \mid (x, z) \in \mathcal{W}\}$,
  its *projection* onto $\mathbb{Z}$: $\mathcal{W}^{\mathbb{Z}} := \{z \mid \exists x \text{ s.t. } (x, z) \in \mathcal{W}\}$.
- For a joint distribution π, define
  its *marginal* onto $\mathbb{Z}$: $\pi^{\mathbb{Z}}(\mathcal{Z}) := \pi(\mathbb{X} \times \mathcal{Z})$,
  its *conditional* $\pi(\mathcal{X}|z) := \frac{\mathrm{d}\pi(\mathcal{X} \times \cdot)}{\mathrm{d}\pi^{\mathbb{Z}}(\cdot)}(z)$ (this is **only $\boldsymbol{\pi}^{\mathbb{Z}}$-a.s. unique**).
- Define "$=^{\xi}$", "$\subseteq^{\xi}$" as the extensions of "$=$", "$\subseteq$" up to a set of ξ-measure-zero.

Theory

Absolutely continuous case

- For any z and x, $\mu(\cdot\,|z)$ and $\nu(\cdot\,|x)$ are either abs. cont. (w.r.t ξ and ζ) or zero.
- Represented by density functions $p(x|z)$ and $q(z|x)$.
- Incl.: "smooth" distr. on Euclidean spaces / manifolds, *all* distr. on finite/discrete spaces.
- Incl.: VAEs, diffusion-based models.

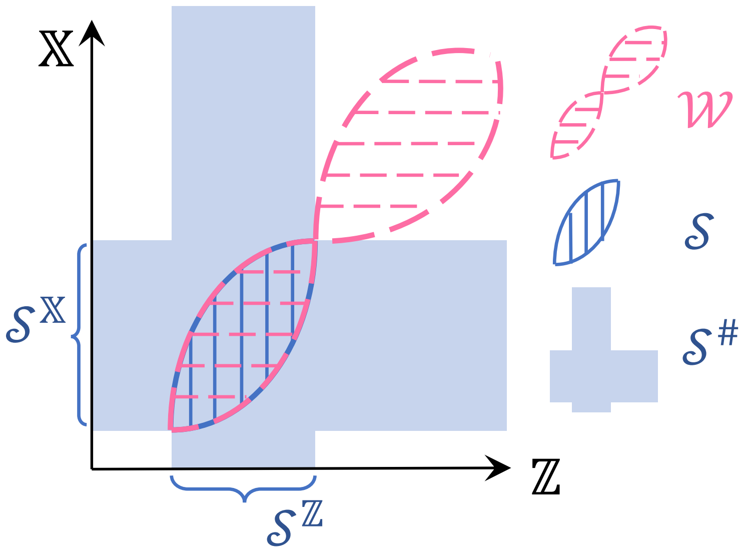
Theory

Absolutely continuous case

- Compatibility
  - First intuition: the ratio $\frac{p(x|z)}{q(z|x)} \overset{\text{when compatible}}{=} \frac{p(x,z)/p(z)}{p(x,z)/p(x)} = p(x)\frac{1}{p(z)}$ factorizes.
  - The classical condition [Arnold'89,01] requires the factorization over $\mathbb{X} \times \mathbb{Z}$:
    It is *not necessary*! Because $p(x|z)$ is uncontrolled outside the support of $\pi^{\mathbb{Z}}$.

  For identifying a proper region for the factorization,

  - **Definition**: A set $\mathcal{S}$ is said to be a $\xi \otimes \zeta$*-complete component* of $\mathcal{W} \in \mathscr{X} \otimes \mathscr{Z}$, **if** $\mathcal{S}^{\#} \cap \mathcal{W} =^{\xi\otimes\zeta} \mathcal{S}$, where
    $\mathcal{S}^{\#} := \mathcal{S}^{\mathbb{X}} \times \mathbb{Z} \cup \mathbb{X} \times \mathcal{S}^{\mathbb{Z}}$ is the *stretch* of $\mathcal{S}$.
    - *Complete* under stretching and intersecting with $\mathcal{W}$: so that integral on $\mathcal{S}_z$ = integral on $\mathcal{W}_z$, for a.e. $z \in \mathcal{S}^{\mathbb{Z}}$.
    - Conditionals are a.s. determined on $\mathcal{S}^{\#}$ if $\mathcal{S}$ is the support of the joint.



Theory

often just a few candidates, so it is *operable*.

If z is in the support of the joint, then $p(x|z)$ determines the distribution on $\mathbb{X} \times \{z\}$, so $q(z|x)$ should respect it (> 0 where $p(x|z)$ is) to avoid *support conflict*.

Absolutely continuous case

- **Theorem** (compatibility criterion, abs. cont.). $p(x|z)$ and $q(z|x)$ are compatible, **if and only if** there *exists* a set $\mathcal{S}$ (called *complete support*) such that:

makes conditionals *normalized*, since $\mathcal{S}_z =^{\xi} (\mathcal{W}_{p,q})_z = \mathcal{P}_z$.

to make the ratio *well-defined*

(i) $\mathcal{S}$ is a $\xi \otimes \zeta$-*complete component* of both $\mathcal{W}_{p,q} := \bigcup_{z:\mathcal{P}_z \subseteq^{\xi} \mathcal{Q}_z} \mathcal{P}_z \times \{z\}$ and $\mathcal{W}_{q,p} := \bigcup_{x:\mathcal{Q}_x \subseteq^{\zeta} \mathcal{P}_x} \{x\} \times \mathcal{Q}_x$,

where $\mathcal{P}_z := \{x \mid p(x|z) > 0\}$, $\mathcal{P}_x := \{z \mid p(x|z) > 0\}$,

and $\mathcal{Q}_z := \{x \mid q(z|x) > 0\}$, $\mathcal{Q}_x := \{z \mid q(z|x) > 0\}$;

for sufficiency; not guaranteed by (i)

(ii) $\mathcal{S}^{\mathbb{X}} \subseteq^{\xi} \mathcal{W}_{q,p}^{\mathbb{X}}$, $\mathcal{S}^{\mathbb{Z}} \subseteq^{\zeta} \mathcal{W}_{p,q}^{\mathbb{Z}}$;

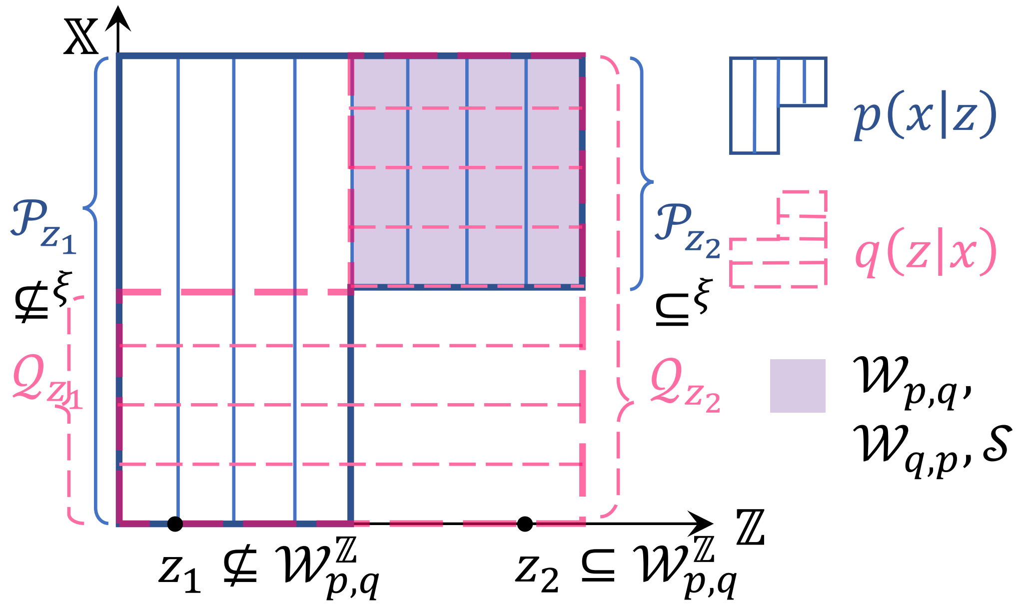
(iii) $(\xi \otimes \zeta)(\mathcal{S}) > 0$;

(iv) $\frac{p(x|z)}{q(z|x)}$ factorizes as $a(x)b(z)$, $\xi \otimes \zeta$-a.e. on $\mathcal{S}$;

the first intuition

(v) $a(x)$ is ξ-integrable on $\mathcal{S}^{\mathbb{X}}$.

For sufficiency, $\pi(\mathcal{W}) := \frac{\int_{\mathcal{W} \cap \mathcal{S}} q(z|x)|a(x)|(\xi \otimes \zeta)(\mathrm{d}x\mathrm{d}z)}{\int_{\mathcal{S}^{\mathbb{X}}} |a(x)|\xi(\mathrm{d}x)}$, $\forall \mathcal{W} \in \mathscr{X} \otimes \mathscr{Z}$ is a compatible joint.



Theory

Absolutely continuous case

- **Theorem** (determinacy, abs. cont.). Let $\mathcal{S}$ be a complete support of *compatible* conditionals $p(x|z)$ and $q(z|x)$. **If** $\mathcal{S}_z =^{\xi} \mathcal{S}^{\mathbb{X}}$ for ζ-a.e. $z \in \mathcal{S}^{\mathbb{Z}}$ or $\mathcal{S}_x =^{\zeta} \mathcal{S}^{\mathbb{Z}}$ for ξ-a.e. $x \in \mathcal{S}^{\mathbb{X}}$, **then** their compatible joint supported on $\mathcal{S}$ is unique.
  - Roughly means $\mathcal{S}$ is "rectangular": *irreducibility* of the Gibbs chain.
  - The uniqueness is only possible on each complete support $\mathcal{S}$.

- **Corollary**. **If** *compatible* conditionals $p(x|z)$ and $q(z|x)$ have a.e.-full supports, **then** their compatible joint on $\mathbb{X} \times \mathbb{Z}$ is unique.
  - Determinacy in the abs. cont. case is often *sufficient*.

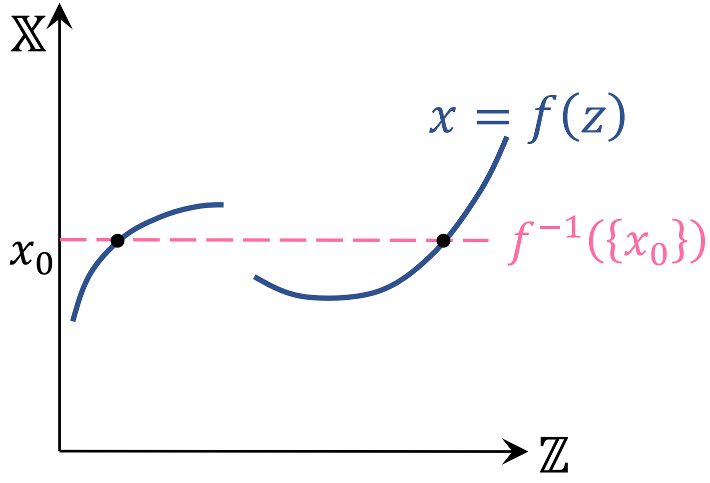
Theory

Dirac case

- $\mu(\mathcal{X}|z) = \delta_{f(z)}(\mathcal{X}) \coloneqq \mathbb{I}[f(z) \in \mathcal{X}]$ ($f: \mathbb{Z} \to \mathbb{X}$ is measurable; e.g., when continuous).
- Incl.: Euclidean/manifold case (no density function), and finite/discrete case (*also abs. cont.*).
- Incl.: GANs, flow-based models.

Compatibility:

- **Theorem** (compatibility criterion, Dirac). Suppose $\mathscr{X}$ contains all the single-point sets. Then conditional $\nu(\cdot|x)$ is compatible with $\mu(\mathcal{X}|z) = \delta_{f(z)}(\mathcal{X})$, **if and only if** there exists $x_0 \in \mathbb{X}$ s.t. $\nu(f^{-1}(\{x_0\})|x_0) = 1$.
  - $\nu(\cdot|x)$ is not required to concentrate on the curve for *any* x: for *one* such x_0, $\delta_{(x_0, f(x_0))}$ is already a compatible joint.



- When $\nu(\cdot|x) \coloneqq \delta_{g(x)}(\cdot)$ and compatibility is desired over a set $\mathcal{X}$:
  - Min the **cycle-consistency loss** $\mathbb{E}_{p(x)} \ell\left(x, f\left(g(x)\right)\right)$ is *sufficient* ($p(x)$ supported on $\mathcal{X}$; ℓ a metric).
  - It is also *necessary* if f is invertible: flow-based models are naturally compatible.

Theory

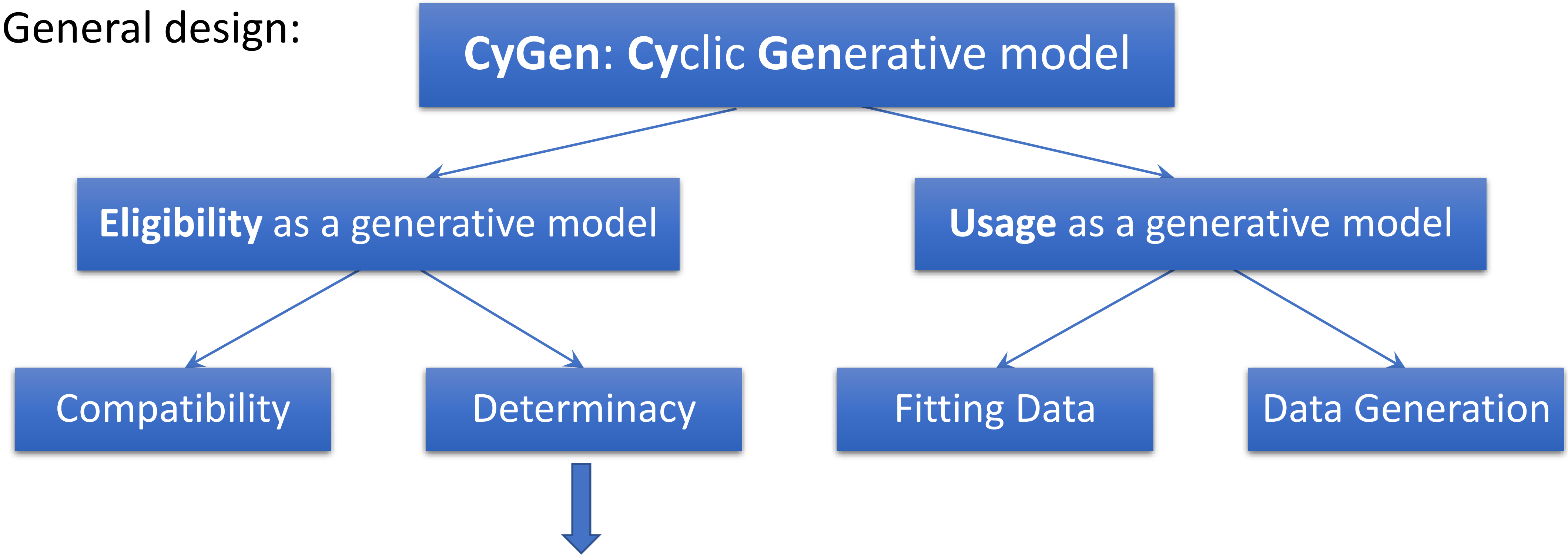
Dirac case

Determinacy:

- On each x_0 in the theorem, there is a compatible joint $\delta_{(x_0, f(x_0))}$.
- But if such an x_0 is not unique, the joint is *not unique* on $\mathbb{X} \times \mathbb{Z}$.
  - Determinacy in the Dirac case is usually *insufficient*:
    Compatible Dirac conditionals only determine a curve on $\mathbb{X} \times \mathbb{Z}$ but not a distribution on it.
  - If $f(z) \equiv x_0$ is constant, then the joint is fully determined by $\nu(\cdot \mid x_0)$.

CyGen

- General design:



- Dirac conditionals (e.g., in GANs, flow-based models) are not suitable (*insufficient* determinacy).
- Use **abs. cont.** conditionals (like VAEs), modeled by parameterized **densities** $p_\theta(x|z)$, $q_\phi(z|x)$ with full supports.

CyGen

- Enforcing compatibility:

  $C(\theta,\phi) := \mathbb{E}_{\rho(x,z)} \left\| \nabla_x \nabla_z^\top r_{\theta,\phi}(x,z) \right\|_F^2$, where $r_{\theta,\phi}(x,z) := \log\left(p_\theta(x|z) / q_\phi(z|x) \right)$,

  and $\rho(x,z)$ is an abs. cont. reference distr. supported on $\mathbb{X} \times \mathbb{Z}$, e.g., $p^*(x) q_\phi(z|x)$.

  - $C(\theta,\phi) = 0 \Leftrightarrow p_\theta(x|z)/q_\phi(z|x)$ factorizes a.e.
  - Generalizes the *cycle-consistency loss* to *probabilistic* conditionals.
  - **Efficient implementation** by Hutchinson's ['89] trace estimator: $\mathrm{tr}(A) = \mathbb{E}_{p(\eta)}[\eta^\top A \eta]$

    ➔ $C(\theta,\phi) = \mathbb{E}_{\rho(x,z)} \mathbb{E}_{p(\eta)} \left\| \nabla_z \left(\eta^\top \nabla_x r_{\theta,\phi}(x,z) \right) \right\|_2^2$.

    #{derivative computation}: $O(d_{\mathbb{X}} d_{\mathbb{Z}})$ ➔ $O(d_{\mathbb{X}} + d_{\mathbb{Z}})$.

    $p(\eta)$ is any distr. s.t. $\mathbb{E}[\eta] = 0$, $\mathrm{Var}[\eta] = I$.

  - Gradient estimation for flows $q_\phi(z|x)$: $z = T_\phi(e|x), e \sim p(e)$ with *intractable inverse*:

    $\nabla_Z \log q_{Z|X}\left(T_\phi(e|x)|x\right) = \left(\nabla_e T_\phi^\top(e|x)\right)^{-1} \nabla_e h_\phi(e,x)$,

    $\nabla_X \log q_{Z|X}\left(T_\phi(e|x)|x\right) = \nabla_x h_\phi(e,x) - \left(\nabla_x T_\phi^\top(e|x)\right) \nabla_Z \log q_{Z|X}\left(T_\phi(e|x)|x\right)$,

    where $h_\phi(e,x) := \log q_{Z|X}\left(T_\phi(e|x)|x\right)$.

CyGen

- Enforcing compatibility:

$$C(\theta,\phi) \coloneqq \mathbb{E}_{\rho(x,z)} \left\| \nabla_x \nabla_z^\top r_{\theta,\phi}(x,z) \right\|_F^2, \text{ where } r_{\theta,\phi}(x,z) \coloneqq \log\left(p_\theta(x|z) / q_\phi(z|x) \right).$$

- Implication on Gaussian VAE $p_\theta(x|z) = \mathcal{N}\left(x \middle| f_\theta(z), \sigma_d^2 I\right)$, $q_\phi(z|x) = \mathcal{N}\left(z \middle| g_\phi(x), \sigma_e^2 I\right)$:

$$C(\theta,\phi) = \mathbb{E}_{\rho(x,z)} \left\| \frac{1}{\sigma_d^2} \left(\nabla_z f^\top(z)\right)^\top - \frac{1}{\sigma_e^2} \nabla_x g^\top(x) \right\|_F^2 = 0 \Longleftrightarrow f_\theta(z), g_\phi(x) \text{ are affine.}$$

  - Meets conclusions in causality [Zhang'09; Peters'14].
  - Root cause of recent observation (latent space is quite linear [Shao'18]) and analysis (latent space coordinates the data manifold [Dai'19], encoder learns a rescaled isometric embedding [Nakagawa'21]).
  - For a nonlinear repr., use a more flexible $q_\phi(z|x)$ model (e.g., Sylvester flow [VDBerg'18]).
- Relation to AE regularizations:
  - Contractive AE [Rifai'11]: $\mathbb{E}_{p^*(x)} \|\nabla g^\top(x)\|_F^2$.
  - Denoising AE [Rifai'11; Alain'14]: $\mathbb{E}_{p^*(x)} \|\nabla (f \circ g)^\top\|_F^2$ (Gauss. enc. noise, infinitesimal Gauss. corruption).
  - "Tied weights" in AEs [Vincent'08; Rifai'11; Alain'14]: compatibility for sigmoid conditionals.

CyGen

- Fitting data:
  - Maximum Likelihood Estimator (MLE) is available:

$$(\max_{\theta,\phi})\ \mathbb{E}_{p^*(x)}[\log p_{\theta,\phi}(x)] = \mathbb{E}_{p^*(x)}\Big[\underbrace{-\log \mathbb{E}_{q_\phi(z'|x)}[1/p_\theta(x|z')]}_{\approx \log \sum_{i=1}^N \exp(-\log p_\theta(x|z^{(i)})) - \log N}\Big].$$

`logsumexp` trick for numerical stability

$\{z^{(i)}\}_{i=1}^N \sim q_\phi(z'|x)$

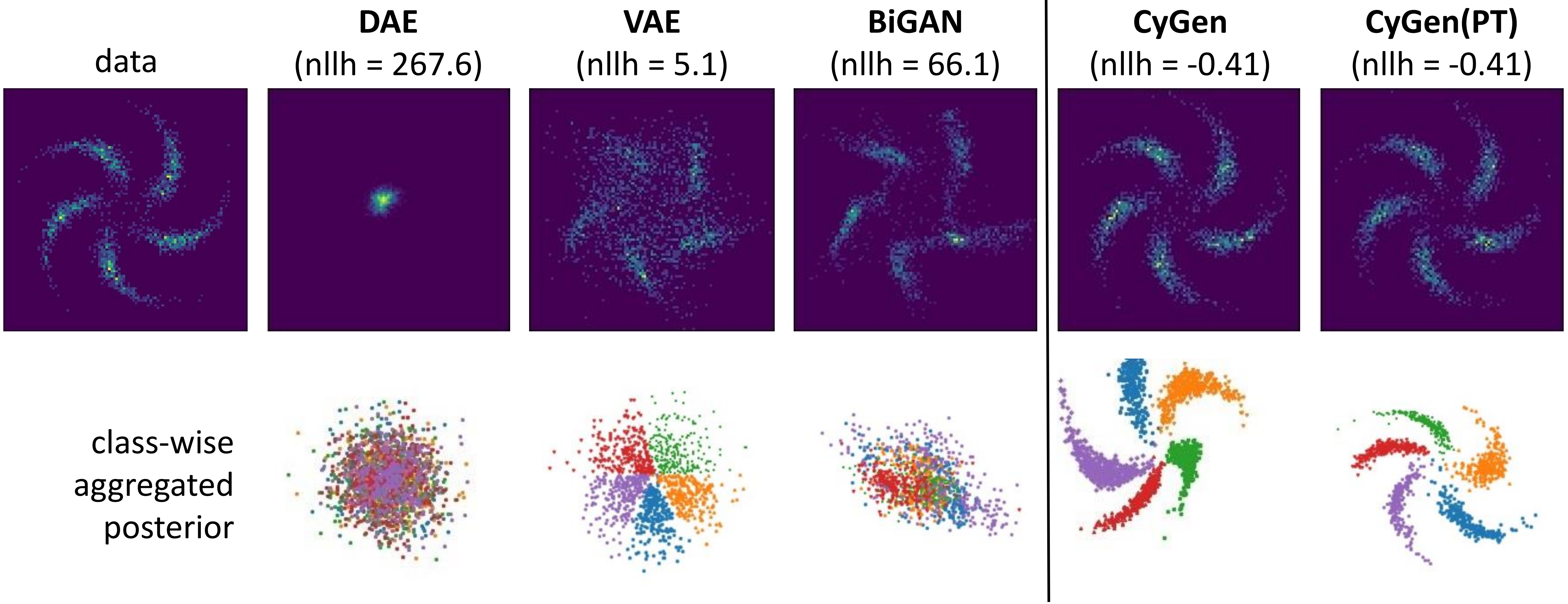
  - The DAE objective $\mathbb{E}_{p^*(x)q_\phi(z'|x)}[\log p_\theta(x|z')] \geq \mathbb{E}_{p^*(x)}[\log p_{\theta,\phi}(x)]$: improper for MLE; makes $q_\phi(z'|x)$ mode-collapsed and hurts determinacy.
  - CyGen final training loss: $(\min_{\theta,\phi})\ \mathbb{E}_{p^*(x)}[-\log p_{\theta,\phi}(x)] + \lambda\, C(\theta,\phi)$.
- Data generation: sample from the model-determined data distribution $p_{\theta,\phi}(x)$.
  - **Dynamics-based MCMCs**:
    - Converge faster than Gibbs sampling.
    - Only need unnormalized $p_{\theta,\phi}(x)$, which is available: $p_{\theta,\phi}(x) \propto \frac{p_\theta(x|z)}{q_\phi(z|x)}, \forall z$.
    - E.g., Stochastic Gradient Langevin dynamics (SGLD):

$$x^{(t+1)} = x^{(t)} + \varepsilon \nabla_{x^{(t)}} \log \frac{p_\theta(x^{(t)}|z^{(t)})}{q_\phi(z^{(t)}|x^{(t)})} + \sqrt{2\varepsilon}\, \eta^{(t)}, \text{ where } z^{(t)} \sim q_\phi(z|x^{(t)}), \eta^{(t)} \sim \mathcal{N}(0, I).$$

Experiment Results: Synthetic

PreTrain as a VAE then mainly finetune $q_\phi(z|x)$.

- **Generation** and **Representation**: *manifold mismatch* and *posterior collapse* solved.



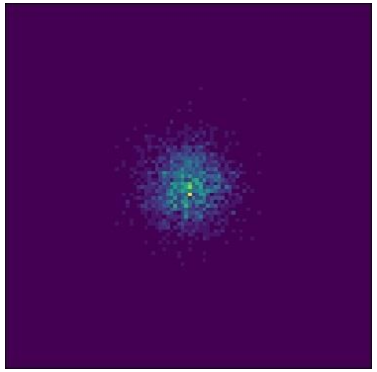
Experiment Results: Synthetic

- **Incorporating knowledge into conditional models**

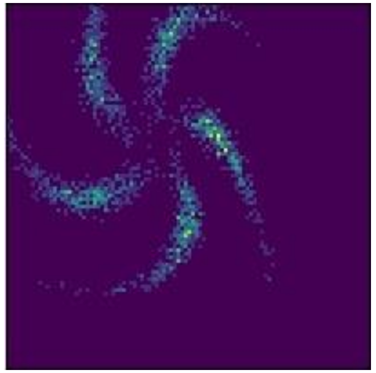
  The VAE-pretrained $p_\theta(x|z)$ model encodes the knowledge:

  "*the prior is centered and centrosymmetric*".

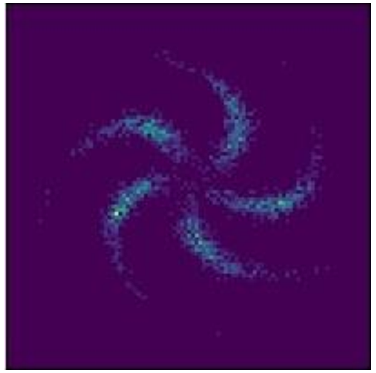
Prior of **VAE**



Prior of **CyGen**



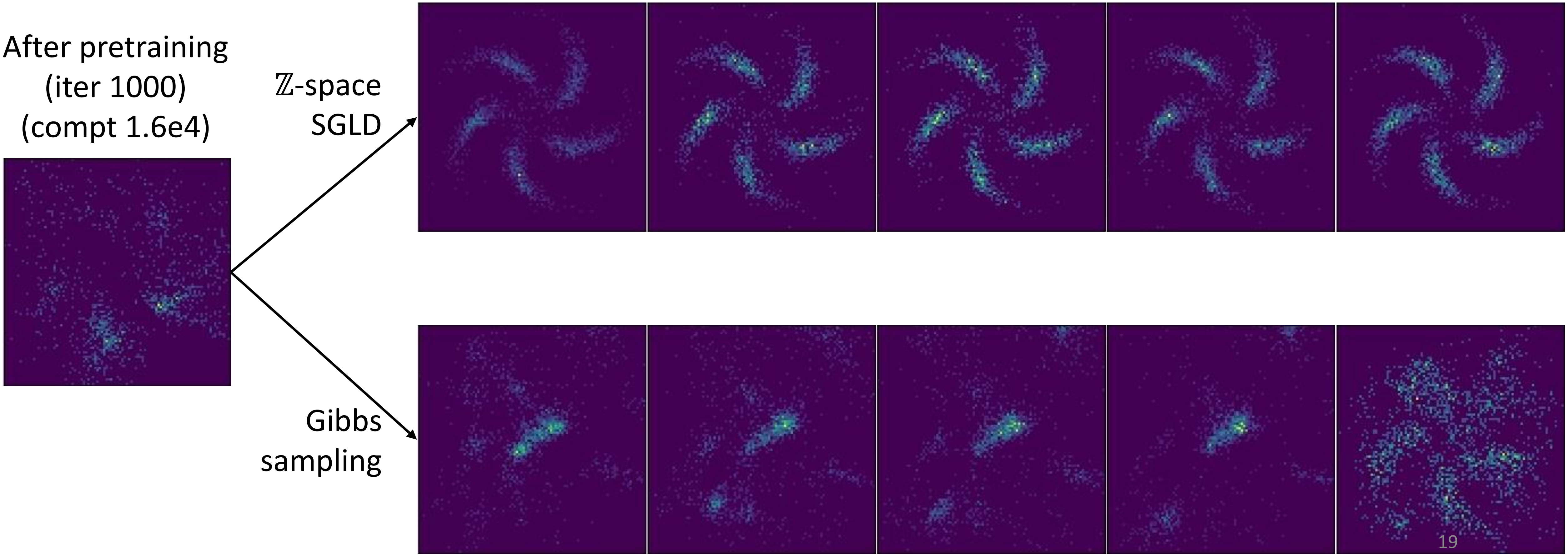
Prior of **CyGen(PT)**



Experiment Results: Synthetic

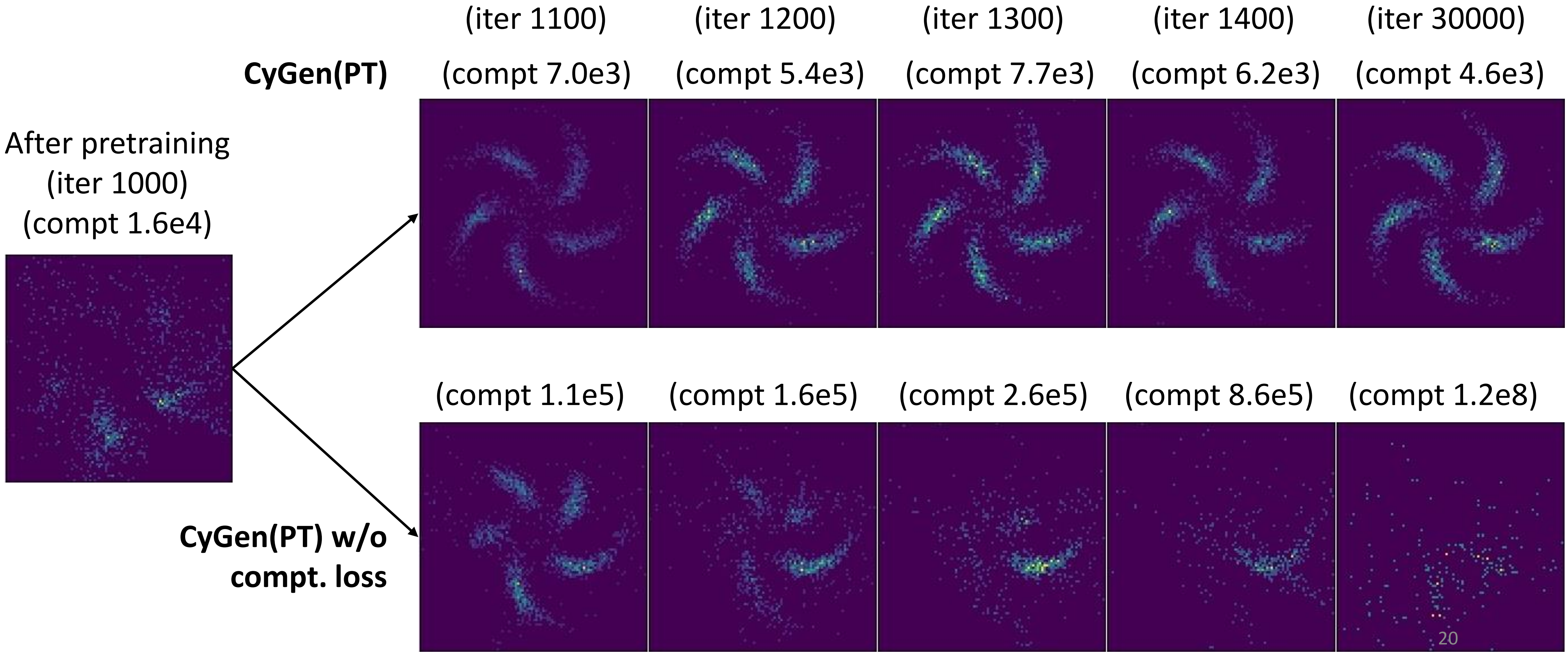
- **Comparison of data generation methods**: SGLD is better and more robust to incompatibility.

CyGen(PT)	(iter 1100)	(iter 1200)	(iter 1300)	(iter 1400)	(iter 30000)
	(compt 7.0e3)	(compt 5.4e3)	(compt 7.7e3)	(compt 6.2e3)	(compt 4.6e3)



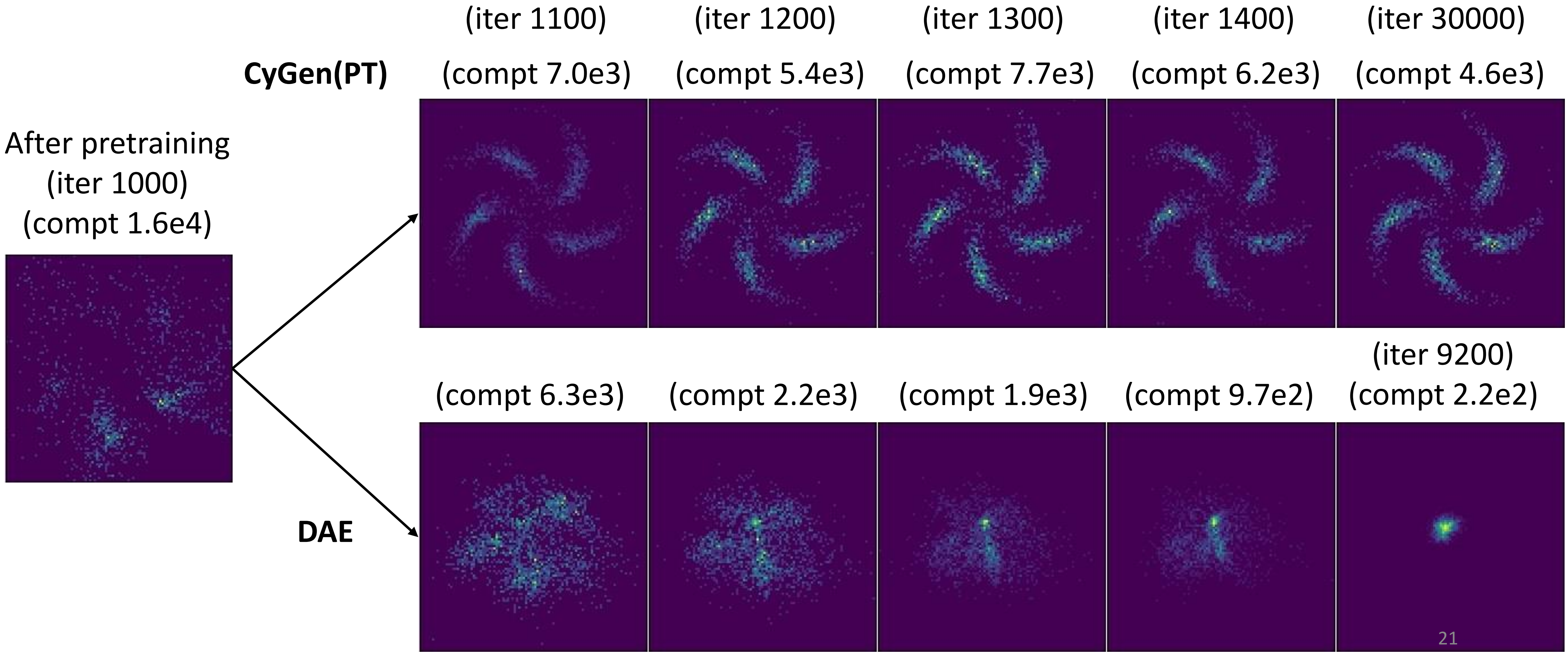
Experiment Results: Synthetic

- **Necessity of compatibility**



Experiment Results: Synthetic

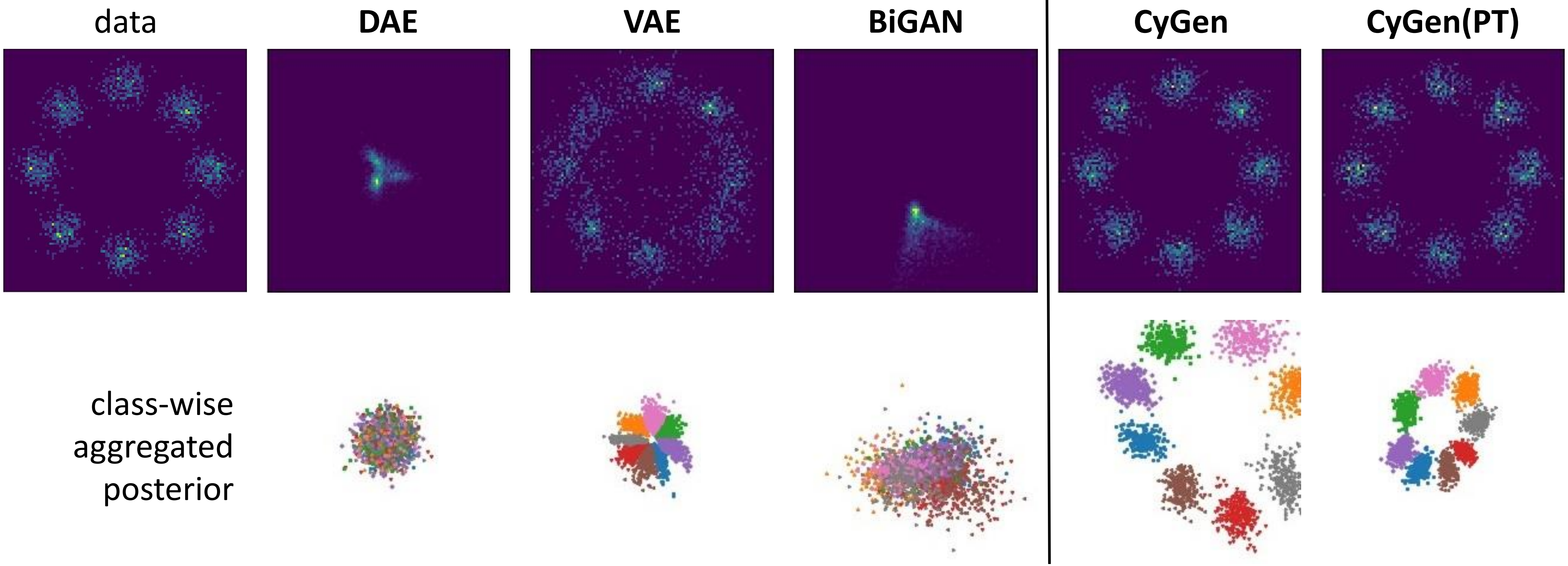
- **DAE mode collapse**



Experiment Results: Synthetic

PreTrain as a VAE then mainly finetune $q_\phi(z|x)$.

- **Generation** and **Representation**: “8gaussians” dataset.



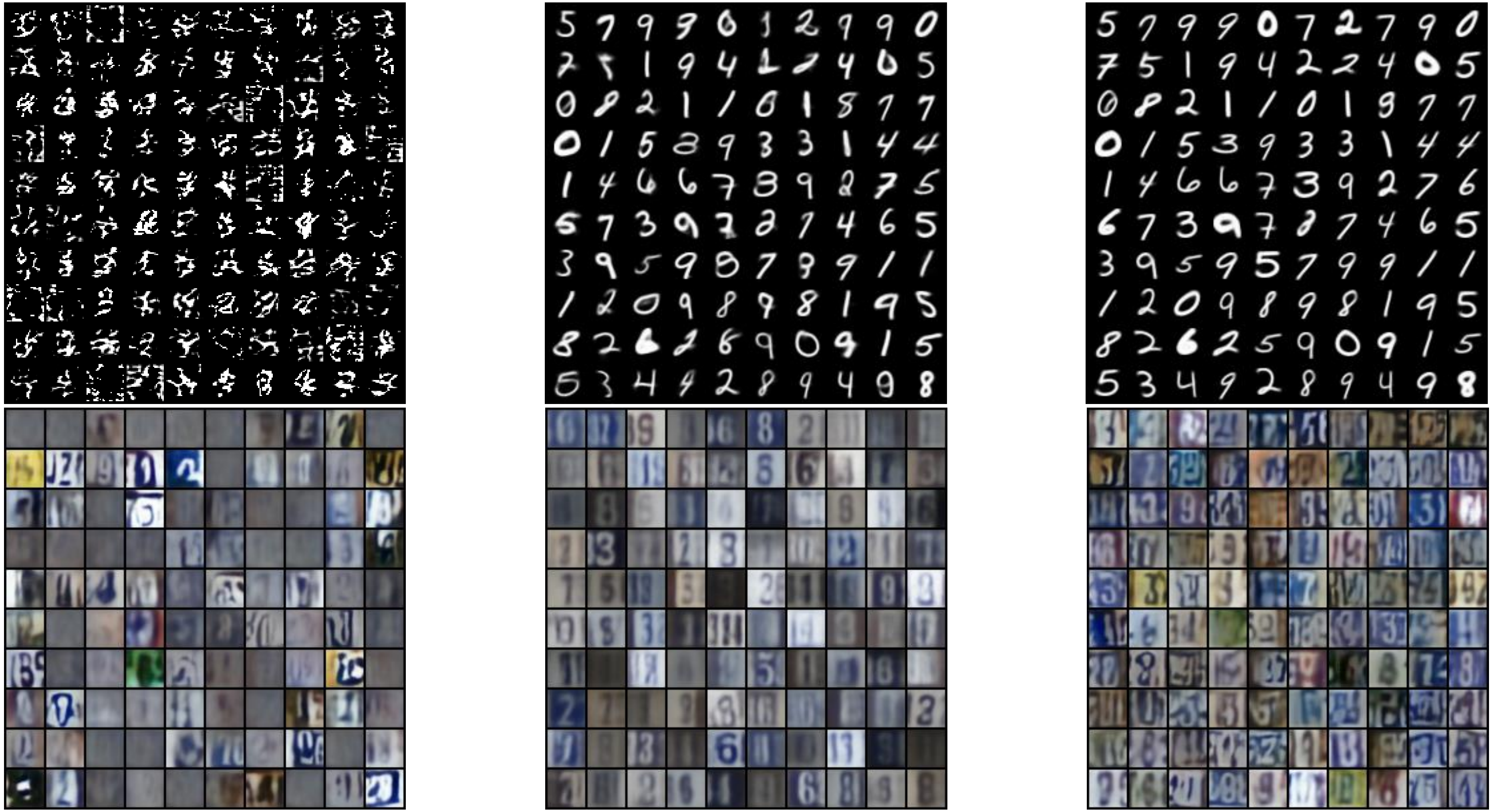
Experiment Results: MNIST & SVHN

- Data generation

DAE | VAE | CyGen(PT)

MNIST

SVHN



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Experiment Results: MNIST & SVHN

- Downstream classification on the latent space:

  A hint on posterior collapse.

  †: Results for BiGAN and GibbsNet are from [Lamb'17] which use a different, deterministic architecture (not suitable for CyGen due to insufficient determinacy).
  They make random guess using the same, probabilistic architecture.

	DAE	VAE	BiGAN†	GibbsNet†	**CyGen**(PT)
MNIST	98.0$\pm$0.1	94.5$\pm$0.3	91.0	97.7	**98.3$\pm$0.1**
SVHN	74.5$\pm$1.0	30.8$\pm$0.2	66.7	**79.6**	**75.8$\pm$0.5**

Thanks!

https://arxiv.org/abs/2106.15962

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