On the Generative Utility of Cyclic Conditionals

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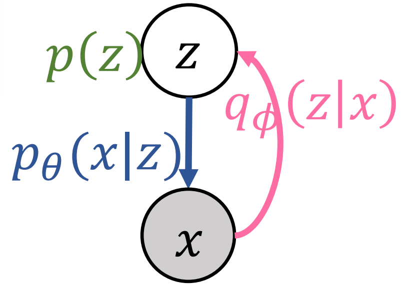
Introduction

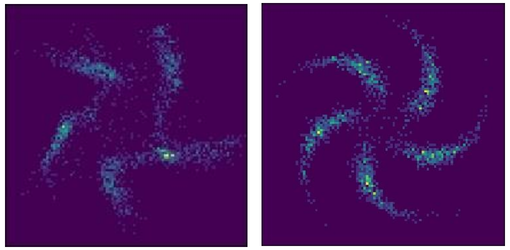
The problem:
Whether or when can we model a *joint* distribution $p(x, z)$
only using two *conditional* models $p(x|z)$ and $q(z|x)$ that form a cycle?



- Motivation from deep generative models:

  Use both a $p(x|z)$ model for *generation*, and a $q(z|x)$ model for *representation*.
  But define their common joint distr. by a prior $p(z)$: $p(x, z) \coloneqq p(z)p(x|z)$.

  - Standard 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.

  - Using an informative prior:

    Domain knowledge on the prior is less common than on the conditional models.
    (e.g., shift/rotation invariance of $q(z|x)$ for image representation (CNN/SphereNet))
  - Learning a prior model: additional cost; harder than learning conditional models.

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, fitting data, and data generation.

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] 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 deterministic conditionals.
- Determinacy
  - Determining $p(x)$ through score matching (SM):
    DAE $\Leftrightarrow$ denoising SM (Gaussian RBM) [Vincent'11].
    DAE $\Leftrightarrow$ 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 $\pi(x|z) \neq p(x|z)$ (depending on the order of vars.) [Heckerman'00, Bengio'13].
    - No explicit expression for learning. Slow convergence for data generation (and learning for Walkback and GibbsNet).

Theory

Setup

- Measure spaces for random variables x and z: $(\mathbb{X}, \mathscr{X}, \xi)$ and $(\mathbb{Z}, \mathscr{Z}, \zeta)$.
- Product measure space $(\mathbb{X} \times \mathbb{Z}, \mathscr{X} \bigotimes \mathscr{Z}, \xi \otimes \zeta)$.
- For $\mathcal{W} \in \mathscr{X} \bigotimes \mathscr{Z}$, define
  its *slice* at z: $\mathcal{W}_z \coloneqq \{x \mid (x, z) \in \mathcal{W}\}$,
  its *projection* onto $\mathbb{Z}$: $\mathcal{W}^{\mathbb{Z}} \coloneqq \{z \mid \exists x \text{ s.t.} (x, z) \in \mathcal{W}\}$.
- For a joint distribution π, define
  its *marginal* onto $\mathbb{Z}$: $\pi^{\mathbb{Z}}(\mathcal{Z}) \coloneqq \pi(\mathbb{X} \times \mathcal{Z})$,
  its *conditional* $\pi(\mathcal{X}|z) \coloneqq \frac{\mathrm{d}\pi(\mathcal{X} \times \cdot)}{\mathrm{d}\pi^{\mathbb{Z}}(\cdot)}(z)$ (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

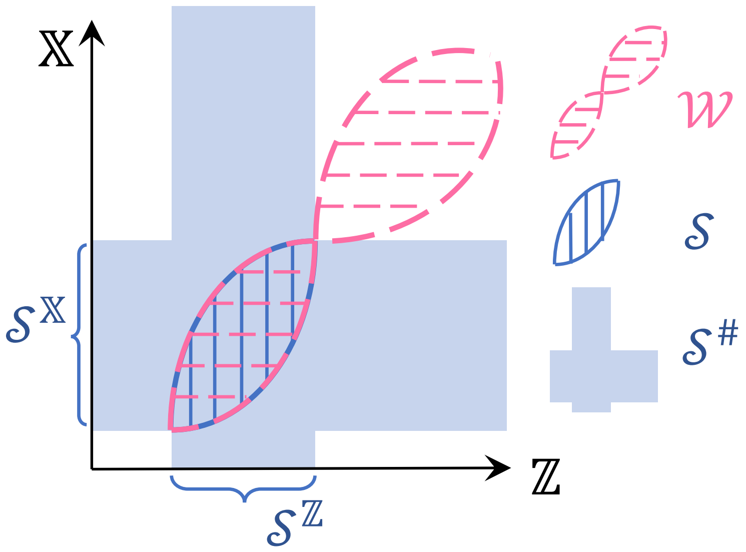
Absolutely continuous case

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

Theory

Absolutely continuous case

- Compatibility
  - First intuition: compatible $\Leftrightarrow$ the ratio $\frac{p(x|z)}{q(z|x)} = \frac{p(x,z)/p(z)}{p(x,z)/p(x)} = p(x)\frac{1}{p(z)}$ 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 integration on $\mathcal{S}_z$ = integration on $\mathcal{W}_z$, for a.e. $z \in \mathcal{S}^{\mathbb{Z}}$. (similarly for $\mathcal{S}_x$, $\mathcal{W}_x$).
    - 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*.

$p(x|z)$ determines the distribution on $\mathbb{X} \times \{z\}$ if z is in the support, 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 $\mathcal{S}_z =^{\xi} (\mathcal{W}_{p,q})_z = \mathcal{P}_z$.

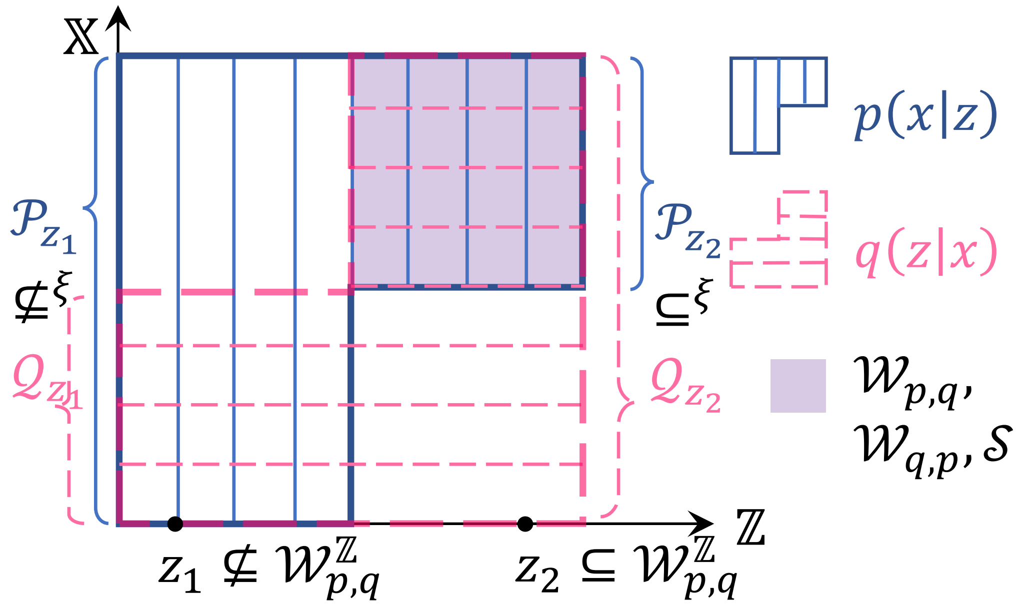
to make the ratio *well-defined*

for sufficiency; not guaranteed by (i)

the first intuition

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

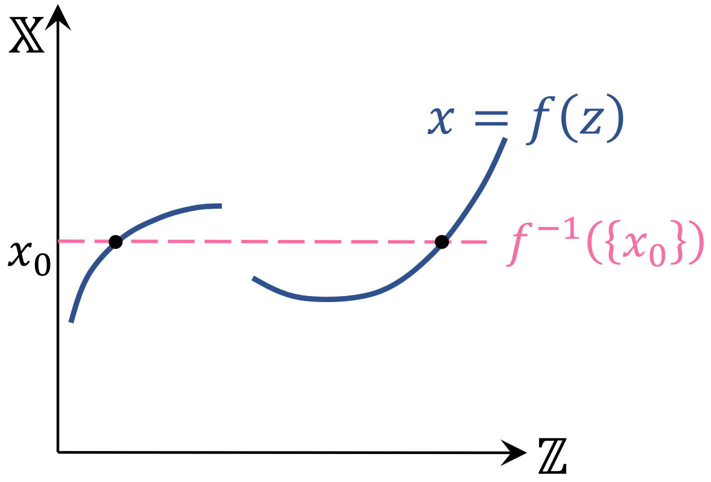
- **Theorem** (determinacy, abs. cont.). Let $\mathcal{S}$ be a complete support of *compatible* conditionals $p(x|z)$ and $q(z|x)$. **If** $\mathcal{S}_z =^{\xi} \mathcal{S}^{\mathbb{X}}$ for ζ-a.e. $z \in \mathcal{S}^{\mathbb{Z}}$ or $\mathcal{S}_x =^{\zeta} \mathcal{S}^{\mathbb{Z}}$ for ξ-a.e. $x \in \mathcal{S}^{\mathbb{X}}$, **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.
- **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 compatibility is desired on a set $\mathcal{X}$ and $\nu(\cdot|x) \coloneqq \delta_{g(x)}(\cdot)$:
  - $\min \mathbb{E}_{p(x)} \ell\Big(x, f\big(g(x)\big)\Big)$ is *sufficient* ($p(x)$ is supported on $\mathcal{X}$; ℓ is a metric): the **cycle-consistency loss** [Kim'17; Zhu'17; Yi'17; Lin'19].
  - It is also *necessary* if f is invertible: flow-based models are naturally compatible.

Theory

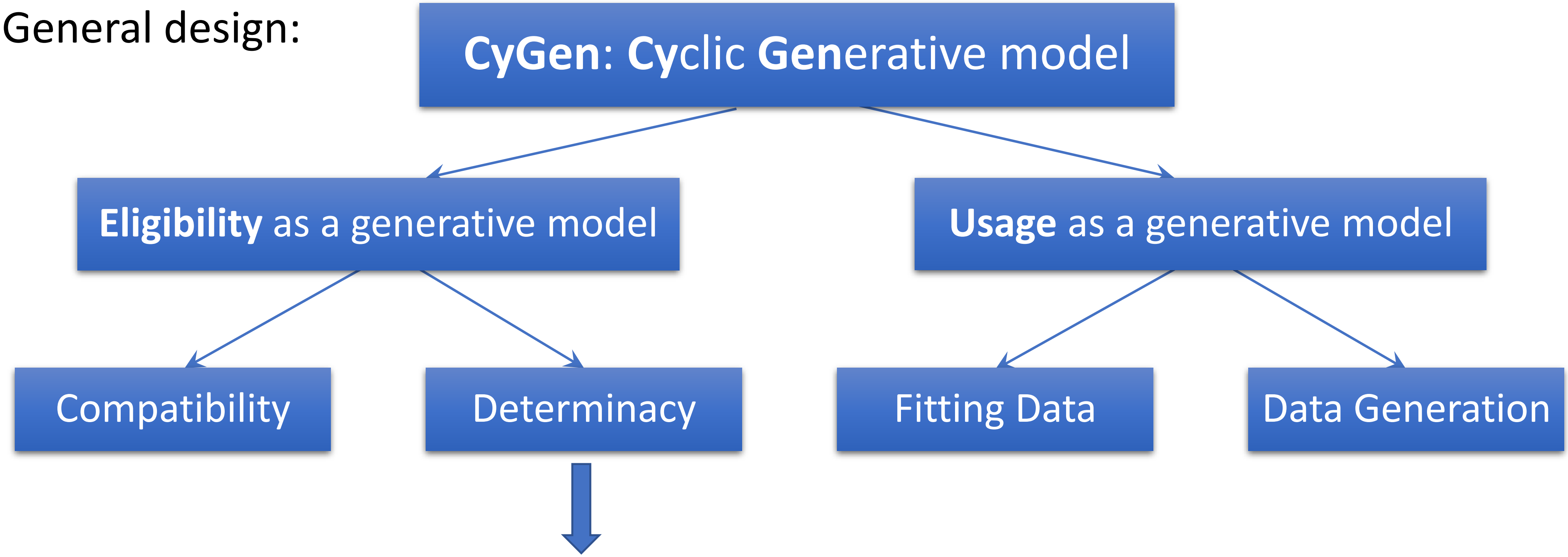
Dirac case

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:



- Use **abs. cont.** conditionals (like VAEs), since Dirac conditionals (like GANs, flow-based models) have *insufficient* determinacy.
- Modeled by parameterized **densities** $p_\theta(x|z)$, $q_\phi(z|x)$ with full supports.

CyGen

- Enforcing compatibility:

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

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

CyGen

- Enforcing compatibility:

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

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

    $C(\theta, \phi) = \mathbb{E}_{\rho(x,z)} \left\| \frac{1}{\sigma_d^2} \left(\nabla_z f^\top(z)\right)^\top - \frac{1}{\sigma_e^2} \nabla_x g^\top(x) \right\|_F^2 = 0 \Longleftrightarrow f_\theta(z), g_\phi(x)$ 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:
  - When compatible, $p_{\theta,\phi}(x) = 1/\int_{\mathbb{Z}} \frac{p_{\theta,\phi}(z')}{p_{\theta,\phi}(x)} \zeta(\mathrm{d}z') = 1/\mathbb{E}_{q_\phi(z'|x)}[1/p_\theta(x|z')]$.
  - Maximum Likelihood Estimate (MLE):
    $$\left(\min_{\theta,\phi}\right)\ \mathbb{E}_{p^*(x)}[-\log p_{\theta,\phi}(x)] = \mathbb{E}_{p^*(x)}\left[\log \mathbb{E}_{q_\phi(z'|x)}[1/p_\theta(x|z')]\right].$$
    - Estimate by \`logsumexp\`.
    - The DAE loss $\mathbb{E}_{p^*(x)q_\phi(z'|x)}[-\log p_\theta(x|z')]$
      - $\leq \mathbb{E}_{p^*(x)}[-\log p_{\theta,\phi}(x)]$: improper for MLE.
      - Makes $q_\phi(z'|x)$ mode-collapsed: hurts determinacy.
  - CyGen final training loss: $\left(\min_{\theta,\phi}\right)\ \mathbb{E}_{p^*(x)}[-\log p_{\theta,\phi}(x)] + \lambda\, C(\theta,\phi)$.

CyGen

- Data generation:

  Sample from the learned data distribution $p_{\theta,\phi}(x)$.

  - **Gibbs sampling**: iteratively sample from $p_\theta(x|z)$ and $q_\phi(z|x)$.
  - **Dynamics-based MCMC**:
    - Converges faster than Gibbs sampling.
    - Only needs an unnormalized density of $p_{\theta,\phi}(x)$, which is available:

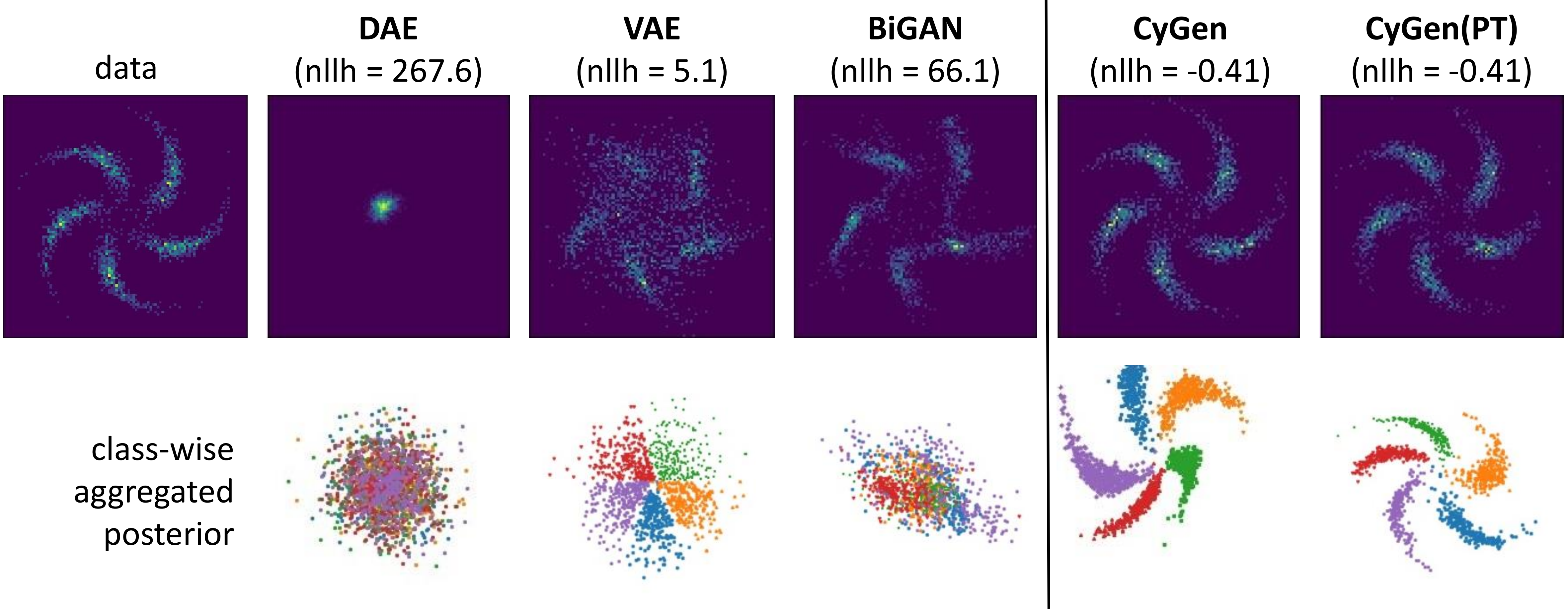
      $p_{\theta,\phi}(x) = \frac{p_{\theta,\phi}(x)}{p_{\theta,\phi}(z)} p_{\theta,\phi}(z) = \frac{p_\theta(x|z)}{q_\phi(z|x)} p_{\theta,\phi}(z) \propto \frac{p_\theta(x|z)}{q_\phi(z|x)}$, for any value of z.
    - E.g., Stochastic Gradient Langevin dynamics (SGLD):

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

Experiment Results: Synthetic

Pre**T**rain as a VAE then mainly finetune $q_\phi(z|x)$.

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



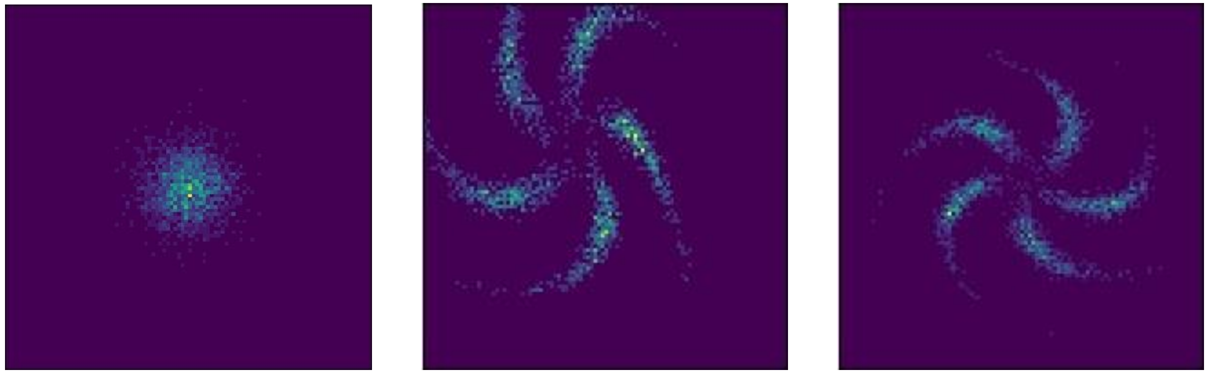
Experiment Results: Synthetic

- **Incorporating knowledge into conditional models**

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

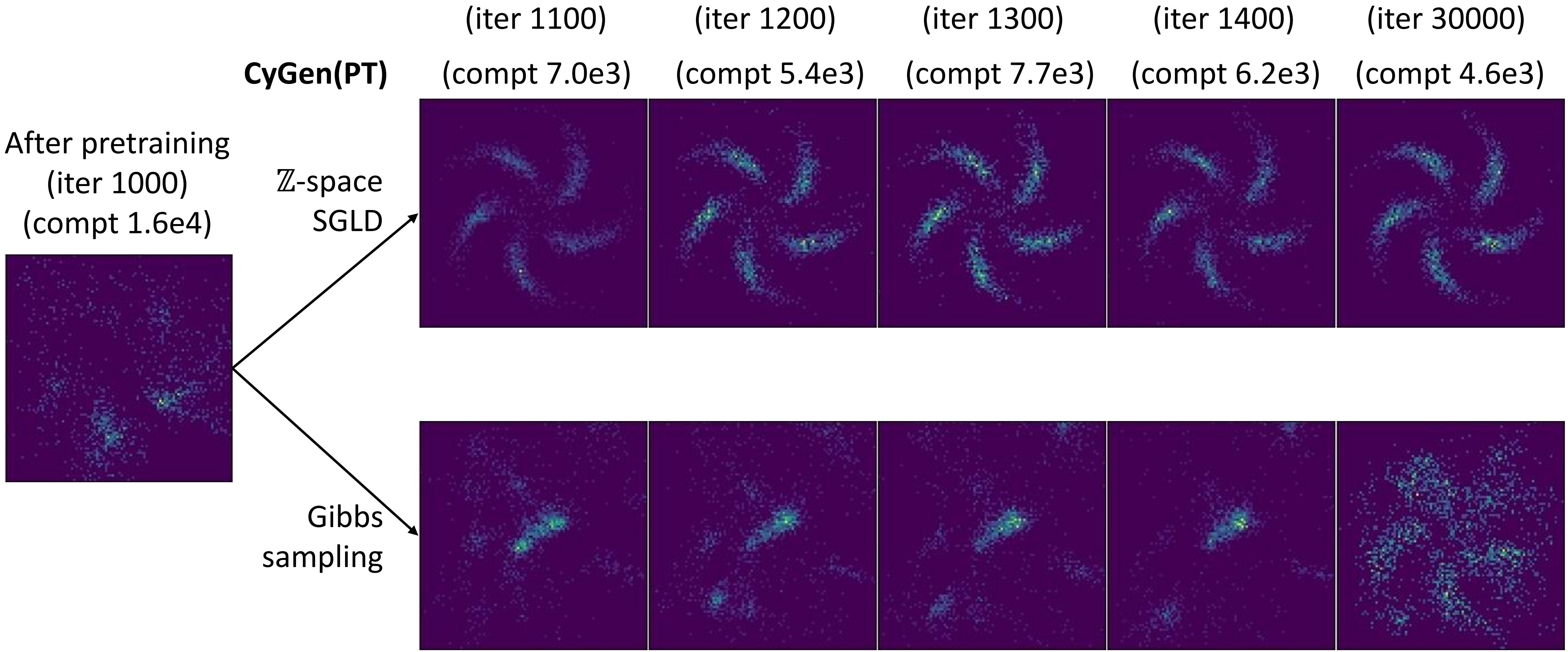
  "the prior is centered and centrosymmetric".

Prior of **VAE** | Prior of **CyGen** | Prior of **CyGen(PT)**



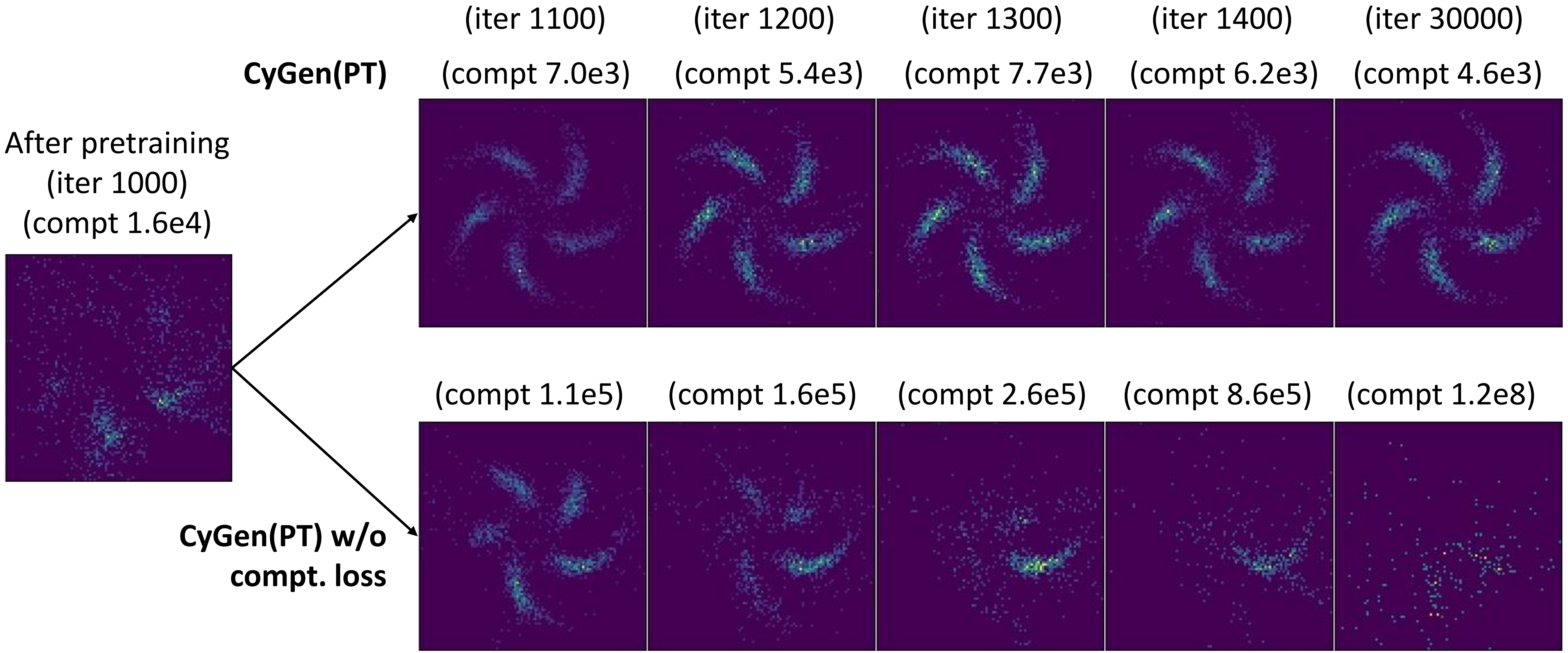
Experiment Results: Synthetic

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



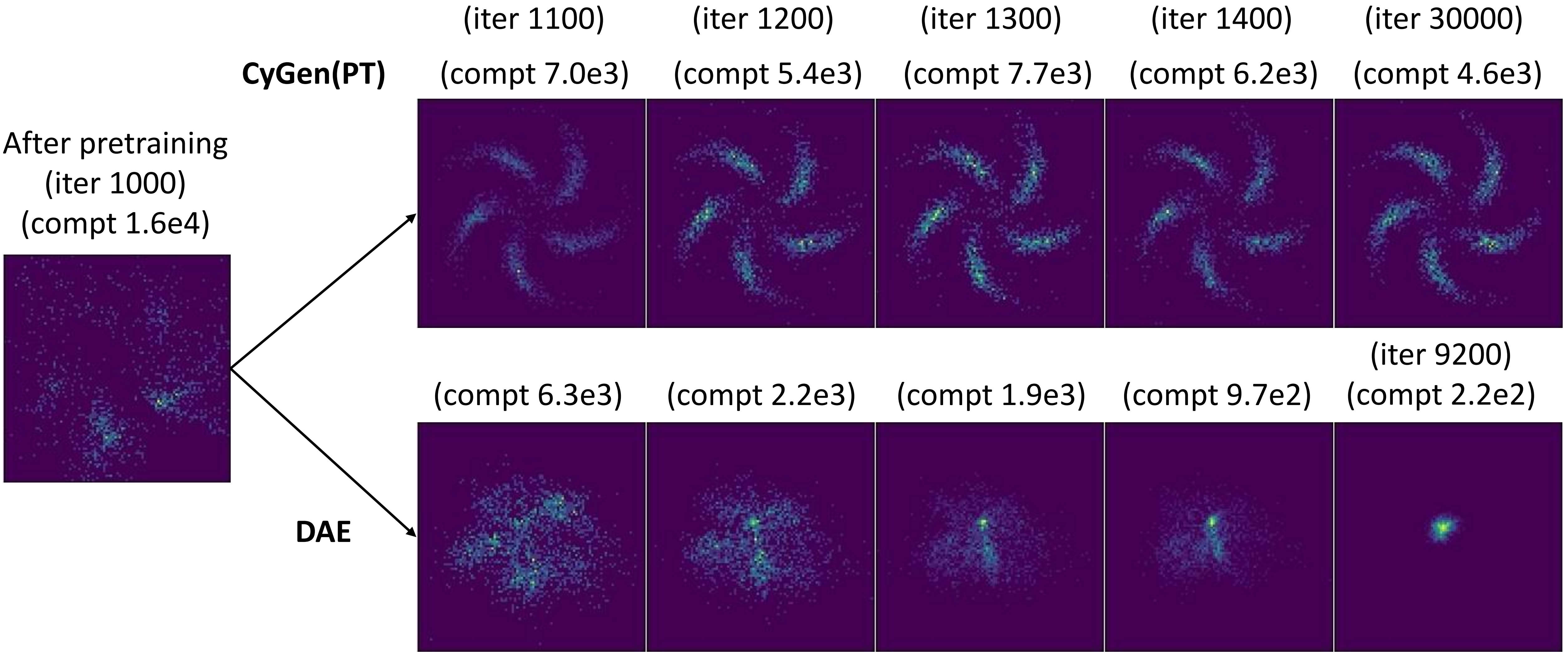
Experiment Results: Synthetic

- **Necessity of compatibility**



Experiment Results: Synthetic

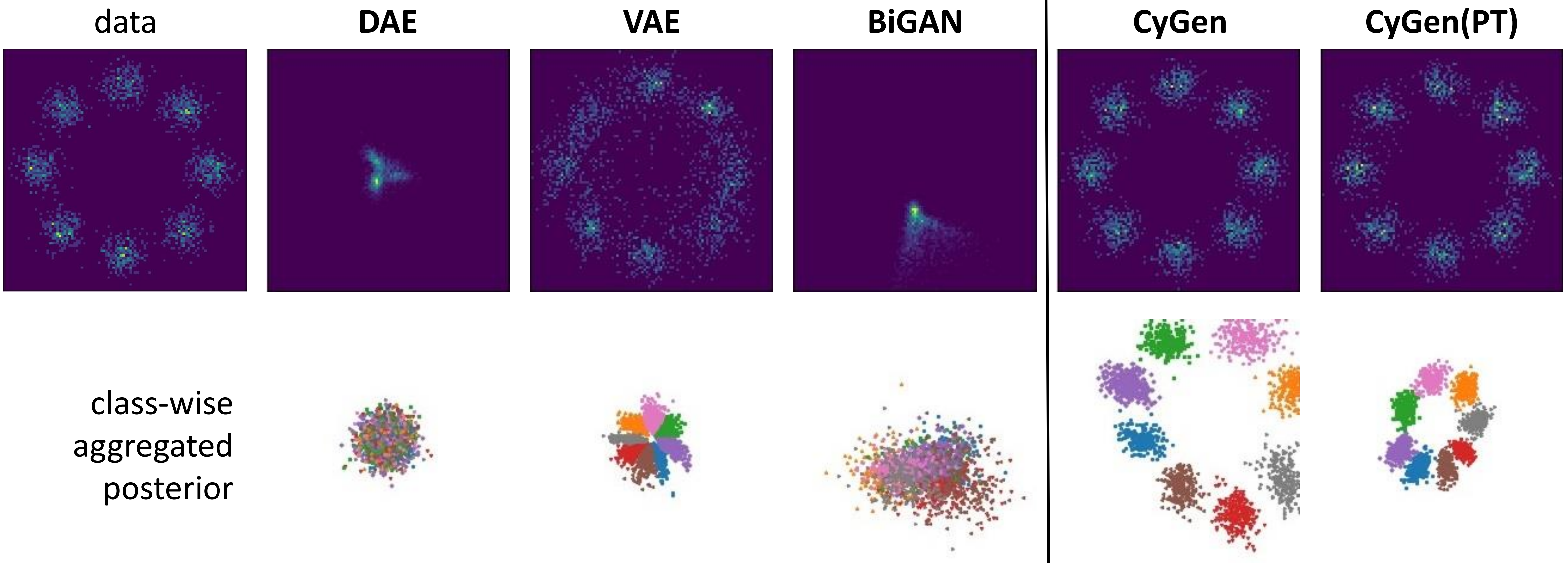
- **DAE mode collapse**



Experiment Results: Synthetic

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

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



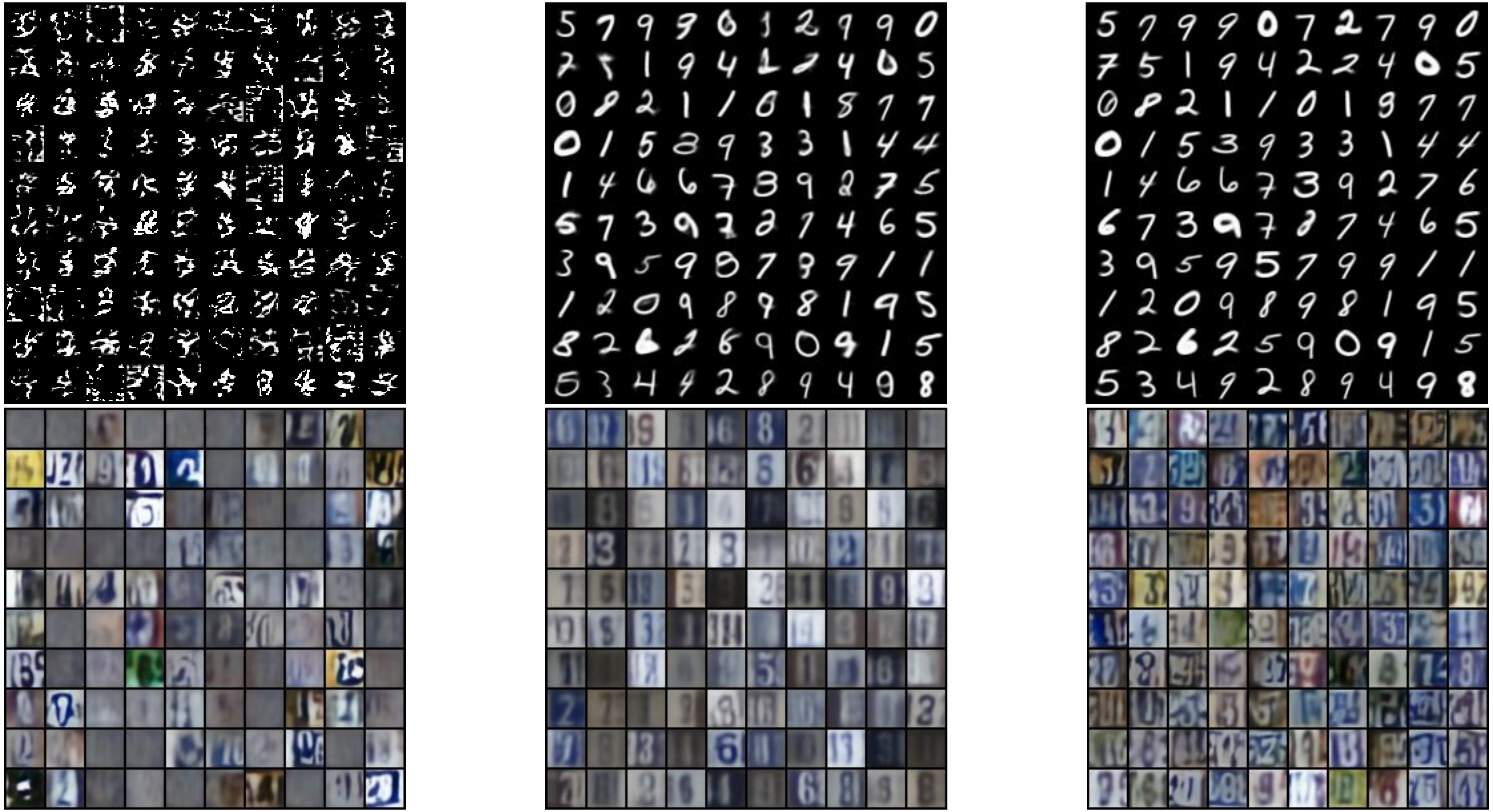
Experiment Results: MNIST & SVHN

- 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.

  - †: For BiGAN and GibbsNet, report the results in [Lamb'17] which use a deterministic architecture (failure using the same architecture).

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

Thanks!

https://arxiv.org/abs/2106.15962

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