On the Generative Utility of Cyclic Conditionals

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Abstract

We study whether and how can we model a joint distribution $p(x, z)$ using two conditional models $p(x|z)$ and $q(z|x)$ that form a cycle. This is motivated by the observation that deep generative models, in addition to a likelihood model $p(x|z)$, often also use an inference model $q(z|x)$ for data representation, but they rely on a usually uninformative prior distribution $p(z)$ to define a joint distribution, which may render problems like posterior collapse and manifold mismatch. To explore the possibility to model a joint distribution using only $p(x|z)$ and $q(z|x)$, we study their *compatibility* and *determinacy*, corresponding to the existence and uniqueness of a joint distribution whose conditional distributions coincide with them. We develop a general theory for novel and operable equivalence criteria for compatibility, and sufficient conditions for determinacy. Based on the theory, we propose the CyGen framework for cyclic-conditional generative modeling, including methods to enforce compatibility and use the determined distribution to fit and generate data. With the prior constraint removed, CyGen better fits data and captures more representative features, supported by experiments showing better generation and downstream classification performance.

1 Introduction

Deep generative models have achieved a remarkable success in the past decade for generating realistic complex data x and extracting useful representations through their latent variable z. Variational auto-encoders (VAEs) [33, 50, 10, 11, 34, 59] follow the Bayesian framework and specify a prior distribution $p(z)$ and a likelihood model $p(x|z)$, so that a joint distribution $p(x, z) = p(z)p(x|z)$ is defined for generative modeling (the joint induces a distribution $p(x)$ on data). An inference model $q(z|x)$ is also used to approximate the posterior distribution $p(z|x)$ (derived from the joint $p(x, z)$), which serves for extracting representations (and learning). Other frameworks like generative adversarial nets [21, 17, 18], flow-based models [16, 44, 32, 22] and diffusion-based models [56, 27, 57, 37] follow the same structure, with different choices of the conditional models $p(x|z)$ and $q(z|x)$ and training objectives. While for the prior $p(z)$, there is often not much knowledge for complex data (like images, text, audio), and these models widely adopt an uninformative prior such as a standard Gaussian. This however, introduces some side effects:

- *Posterior collapse* [11, 25, 47]: The standard Gaussian prior tends to squeeze $q(z|x)$ towards the origin for all x, which degrades the representativeness of the inferred z for x and hurts downstream tasks in the latent space like classification and clustering.
- *Manifold mismatch* [15, 19, 29]: Typically the likelihood model is continuous (keeps topology), so the standard Gaussian prior would restrict the modeled data distribution to a simply-connected support, which limits the capacity for fitting data from a non-(simply) connected support.

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While there are works trying to mitigate the two problems, they require either a strong domain knowledge [36, 40, 29] or a complicated prior model [43].

One question then naturally emerges: *Can we model a joint distribution $p(x, z)$ only using the likelihood $p(x|z)$ and inference $q(z|x)$ models?* If we can, the limitations from the prior issue are then removed from the root. Also, the inference model $q(z|x)$ is then no longer a struggling approximation to a predefined posterior but participate in defining the joint distribution. Modeling conditionals is also argued to be much easier than modeling marginal distributions or the joint directly [1, 6, 7]. In some cases, one may even have better knowledge on the conditionals than on the prior, *e.g.* shift/rotation invariance of image representations (CNNs [39] / SphereNet [13]), and rules to extract frequency/energy features for audio [48]. It is then more natural and effective to incorporate this knowledge into the conditionals than using an uninformative prior.

In this paper, we explore such a possibility, and develop a systematic theory and a CyGen algorithmic framework for **Cy**clic-conditional **Gen**erative modeling. Theoretical analysis on the question breaks down into two sub-problems: when can two given cyclic conditionals correspond to a common joint, and when can they determine the joint. We term them *compatibility* and *determinacy* respectively, corresponding to the existence and uniqueness of a joint that induces the given conditionals. For this, we develop novel compatibility criteria and sufficient conditions for determinacy. In contrast to existing works, our results are operable (vs. existential [8]) and self-contained (vs. requiring a marginal [6, 38]), and are general enough to cover both continuous and discrete cases. Our compatibility criteria are also equivalence (vs. unnecessary [2, 3]) conditions. The theory also enables practical algorithms for CyGen. We propose learning methods to enforce compatibility and fit the determined distribution to data, as well as data generation methods. Techniques for efficient implementation are designed. Note the theory and methods show CyGen determines a flexible prior implicitly, but an explicit model for it is not needed (vs. [43]). We show the practical utility of CyGen in both synthetic and real-world tasks, where the improved performance in downstream classification and data generation demonstrates the advantage to mitigate posterior collapse and manifold mismatch.

1.1 Related work

Denoising auto-encoders (DAEs). Auto-encoders [54, 4] aim to extract data features using a pair of encoder and decoder. In the standard version, they use a deterministic encoder or decoder, which has insufficient determinacy for generative modeling (see Sec. 2.2.2). DAEs [61, 6, 7] use a probabilistic encoder and decoder for robust reconstruction against random data corruption. Their utility as a generative model is first noted through the equivalence to score matching (implying the utility for $p(x)$) for a Gaussian RBM [60] or an infinitesimal Gaussian corruption [1]. In more general cases, the utility to modeling the joint $p(x, z)$ is studied via the Gibbs chain, *i.e.* the Markov chain with transition kernel $p(x'|z')q(z'|x)$. Under a global [6, 38, 23] or local [7] shared support condition, the stationary distribution $\pi(x, z)$ of the Markov chain exists uniquely. But this approach to determining the joint does not give an explicit expression (thus intractable likelihood evaluation), and requires a large number of steps for the chain to converge for data generation and even for learning (Walkback [6], GibbsNet [38]). As for compatibility, it is not really covered in DAEs. Existing results only consider the statistical consistency (unbiasedness under infinite data) of the $p(x|z)$ estimator by fitting (x, z) data from $p^*(x)q(z|x)$ [6, 7, 38, 23], where $p^*(x)$ denotes the true data distribution. Particularly, they require a marginal $p^*(x)$ in advance, so that the joint is already defined by $p^*(x)q(z|x)$ regardless of $p(x|z)$, while compatibility (as well as determinacy) is a matter only of the two conditionals.

More crucially, the DAE loss is not proper for optimizing the encoder $q(z|x)$ as it promotes a mode-collapse behavior. This hinders both compatibility and determinacy (see Sec. 3.2): one may not safely use $q(z|x)$ for inference, and data generation may strongly depend on initialization. In contrast, CyGen does not hinder determinacy by design, and explicitly enforces compatibility. It also enables likelihood evaluation and more efficient data generation.

Dual learning considers conversion tasks between two modalities in both directions, *e.g.*, machine translation [24, 64, 63] and image style transfer [30, 67, 65, 41]. Although we also consider both directions (generation and inference), the fundamental distinction is that in generative modeling there is no data of the latent variable z (not even unpaired). Technically, they did not consider determinacy: they require an external marginal from either a model or data to determine a joint. In fact, determinacy is insufficient for deterministic conversions (see Sec. 2.2.2). Their cycle-consistency loss [30, 67, 65] is a version of our compatibility criterion in a specific Dirac case (see Sec. 2.2.1), and we extend the loss to the more general absolutely continuous case (allowing probabilistic conversion) (see Sec. 3.1).

2 Compatibility and Determinacy Theory

To be a generative model, a system needs to determine a distribution on the data variable x, and with a latent variable z, this amounts to determining a joint distribution on (x, z). This leads to the goal of the analysis on the compatibility and determinacy of cyclic conditionals. In this section we carry out theoretical analysis on the conditions for compatibility and determinacy, which also inspires our novel CyGen framework for generative modeling. We begin with formalizing the problems.

Setup. In this work we focus on cyclic conditionals on two random variables x and z (extension to more variables follows a similar way). Following the convention in machine learning, we call a "probability measure" as a "distribution", and call a "probability density/mass function" as a "density function". Denote the measure spaces of x and z as $(\mathbb{X}, \mathscr{X}, \xi)$ and $(\mathbb{Z}, \mathscr{Z}, \zeta)$[2], where $\mathscr{X}$, $\mathscr{Z}$ are the respective sigma-fields, and the base measures ξ, ζ (*e.g.*, Lebesgue measure on Euclidean spaces, counting measure on finite/discrete spaces) are sigma-finite (unnecessarily finite). We use $\mathcal{X} \in \mathscr{X}$, $\mathcal{Z} \in \mathscr{Z}$ to denote measurable sets, and use "$\stackrel{\xi}{=}$", "$\stackrel{\xi}{\subseteq}$" as the extensions of "$=$", "$\subseteq$" up to a set of ξ-measure-zero (Def. A.1). Note that we do not require any further structures such as topology, metric, or linearity, for the interest of the most general conclusions that unify Euclidean/manifold and finite/discrete spaces and allow $\mathbb{X}$, $\mathbb{Z}$ with different dimensions or types.

Joint and conditional distributions are defined on the product measure space $(\mathbb{X}\times\mathbb{Z}, \mathscr{X}\otimes\mathscr{Z}, \xi\otimes\zeta)$, where "$\times$" is the usual Cartesian product, $\mathscr{X}\otimes\mathscr{Z} := \sigma(\mathscr{X}\times\mathscr{Z})$ is the sigma-field generated by measurable rectangles from $\mathscr{X}\times\mathscr{Z}$, and $\xi\otimes\zeta$ is the product measure [9, Thm. 18.2]. Define the *slice* of $\mathcal{W} \in \mathscr{X}\otimes\mathscr{Z}$ at z as $\mathcal{W}_z := \{x \mid (x, z) \in \mathcal{W}\}$ [9, Thm. 18.1(i)], and its *projection* onto $\mathbb{Z}$ as $\mathcal{W}^{\mathbb{Z}} := \{z \mid \exists x \in \mathbb{X} \text{ s.t. } (x, z) \in \mathcal{W}\} \in \mathscr{Z}$ (Appx. A.3). Similarly denote the *marginal* of a joint π on $\mathbb{Z}$ as $\pi^{\mathbb{Z}}(\mathcal{Z}) := \pi(\mathbb{X}\times\mathcal{Z}), \forall\mathcal{Z} \in \mathscr{Z}$ in a similar style. To keep the same level of generality, we follow the general definition of conditionals: $\forall\mathcal{X} \in \mathscr{X}$, the conditional $\pi(\mathcal{X}|z)$ of joint π is the density function (Radon-Nikodym derivative) of $\pi(\mathcal{X}\times\cdot)$ w.r.t $\pi^{\mathbb{Z}}$ ([9, p.457]; see also Appx. A.4). We highlight the key characteristic under this generality that $\pi(\cdot|z)$ can be arbitrary on a set of $\pi^{\mathbb{Z}}$-measure-zero, particularly, outside the support of $\pi^{\mathbb{Z}}$. Appx. A provides more background on measure theory. The goals of the analysis can be then formalized below.

Definition 2.1 (compatibility and determinacy)**.** We say two conditionals $\mu(\mathcal{X}|z)$, $\nu(\mathcal{Z}|x)$ are *compatible*, if there exists a joint distribution π on $(\mathbb{X}\times\mathbb{Z}, \mathscr{X}\otimes\mathscr{Z})$ such that $\mu(\mathcal{X}|z)$ and $\nu(\mathcal{Z}|x)$ are its conditional distributions. We say two compatible conditionals have *determinacy* on a set $\mathcal{S} \in \mathscr{X}\otimes\mathscr{Z}$, if there is only one joint distribution concentrated on $\mathcal{S}$ that makes them compatible.

We now analyze the conditions for compatibility and determinacy in the absolutely continuous and the Dirac cases. Distributions have qualitatively different behaviors in the two cases, and they correspond to different types of generative models. Note that the concepts only involve the two conditionals, so we desire conditions free of any marginal or joint distributions (vs. DAE results).

2.1 Absolutely Continuous Case

We first consider the case where for any $z \in \mathbb{Z}$ and any $x \in \mathbb{X}$,[3] the conditionals $\mu(\cdot|z)$ and $\nu(\cdot|x)$ are either absolutely continuous (w.r.t ξ and ζ, resp.) [9, p.448], or zero in the sense of a measure. This is equivalent to that they have density functions $p(x|z)$ and $q(z|x)$ (non-negative by definition; may integrate to zero), including "smooth" distributions on Euclidean spaces or manifolds, as well as *all* distributions on finite/discrete spaces. We also refer to such a conditional by its density. As conditional models are often specified in the form of density, this case covers many generative model frameworks, notably VAEs [33, 50, 49, 34, 59] and diffusion-based models [56, 27, 57].

2.1.1 Compatibility criterion in the absolutely continuous case

To put the concept into practical use, we need an operable criterion to tell the compatibility of two given conditionals. In the absolutely continuous case, one may expect that when $p(x|z)$ and $q(z|x)$ are compatible, the joint is also absolutely continuous (w.r.t $\xi\otimes\zeta$) with some density $p(x, z)$. This intuition is verified by Lem. C.1 in Appx. C.1. For a sloppy inspiration, one could then safely apply density-function calculus and get $\frac{p(x|z)}{q(z|x)} = \frac{p(x,z)}{p(z)} / \frac{p(x,z)}{p(x)} = \frac{p(x)}{p(z)}$ factorizes into a function of x and a function of z. Conversely, if the ratio factorizes as such $\frac{p(x|z)}{q(z|x)} = a(x)b(z)$, one could get

[2] The symbol $\mathbb{Z}$ overwrites the symbol for the set of integers, which is not involved in this paper.

[3] There may be problems if absolute continuity holds only for ζ-a.e. z and ξ-a.e. x; see Appx. Example C.2.

$p(x|z)\frac{1}{Ab(z)} = q(z|x)\frac{a(x)}{A}$ where $A := \int_{\mathbb{X}} a(x)\xi(\mathrm{d}x)$, which defines a joint density and compatibility is achieved. This intuition leads to the classical compatibility criterion [2, Thm. 4.1; 3, Thm. 1].

However, it is more complicated than imagined. Berti et al. [8, Example 9] point out that the classical criterion is only sufficient but *not necessary*. The subtlety is about on which region does this factorization have to hold. The classical criterion requires it to be the positive region of $p(x|z)$ and also coincide with that of $q(z|x)$. But as mentioned, conditional $\mu(\cdot|z)$ can be arbitrary outside the support of the marginal $\pi^{\mathbb{Z}}$ (similarly for $\nu(\cdot|x)$), which may lead to additional positive regions that violate the requirement.[4] To address the problem, Berti et al. [8] give an equivalence criterion (Thm. 8), but it is *existential* thus less useful as the definition of compatibility is itself existential. Moreover, these criteria are restricted to either Euclidean or discrete spaces.

Next we give our *equivalence* criterion that is *operable*. In addressing the subtlety with regions, we first introduce a related concept that helps identify appropriate regions.

Definition 2.2 ($\xi \otimes \zeta$-complete component)**.** For a set $\mathcal{W} \in \mathscr{X} \otimes \mathscr{Z}$, we say that a set $\mathcal{S} \in \mathscr{X} \otimes \mathscr{Z}$ is a *$\xi \otimes \zeta$-complete component* of $\mathcal{W}$, if $\mathcal{S}^\sharp \cap \mathcal{W} \overset{\xi \otimes \zeta}{=} \mathcal{S}$, where $\mathcal{S}^\sharp := \mathcal{S}^{\mathbb{X}} \times \mathbb{Z} \cup \mathbb{X} \times \mathcal{S}^{\mathbb{Z}}$ is the *stretch* of $\mathcal{S}$.

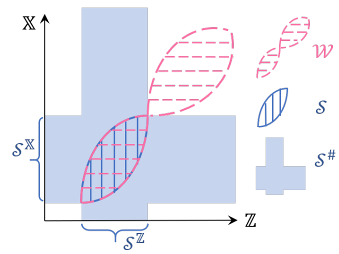

Figure 1: Illustration of a $\xi \otimes \zeta$-complete component $\mathcal{S}$ of $\mathcal{W}$.

Fig. 1 illustrates the concept. Roughly, the stretch $\mathcal{S}^\sharp$ of $\mathcal{S}$ represents the region where the conditionals are a.s. determined if $\mathcal{S}$ is the *support*[5] of the joint. If $\mathcal{S}$ is a complete component of $\mathcal{W}$, it is complete under stretching and intersecting with $\mathcal{W}$. Such a set $\mathcal{S}$ is an a.s. subset of $\mathcal{W}$ (Lem. B.12), while has a.s. the same slice as $\mathcal{W}$ does for almost all $z \in \mathcal{S}^{\mathbb{Z}}$ and $x \in \mathcal{S}^{\mathbb{X}}$ (Lem. B.16). This is critical for the normalizedness of distributions in our criterion. Appx. B.3 shows more facts. With this concept, our compatibility criterion is presented below.

Theorem 2.3 (compatibility criterion, absolutely continuous)**.** *Let $p(x|z)$ and $q(z|x)$ be the density functions of two everywhere absolutely continuous (or zero) conditional distributions, and define:*

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

Then they are compatible, if and only if they have a complete support $\mathcal{S}$, *defined as a **(i)** $\xi \otimes \zeta$-complete component of both*

$$\mathcal{W}_{p,q} := \bigcup_{z : \mathcal{P}_z \subseteq^\xi \mathcal{Q}_z} \mathcal{P}_z \times \{z\}, \; \mathcal{W}_{q,p} := \bigcup_{x : \mathcal{Q}_x \subseteq^\zeta \mathcal{P}_x} \{x\} \times \mathcal{Q}_x,$$

*such that: **(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)** $(\xi \otimes \zeta)(\mathcal{S}) > 0$, and **(iv)** $\frac{p(x|z)}{q(z|x)}$ factorizes as $a(x)b(z)$, $\xi \otimes \zeta$-a.e. on $\mathcal{S}$,*[6] *where **(v)** $a(x)$ is ξ-integrable on $\mathcal{S}^{\mathbb{X}}$. For sufficiency,*

$$\pi(\mathcal{W}) := \frac{\int_{\mathcal{W} \cap \mathcal{S}} q(z|x) |a(x)| (\xi \otimes \zeta)(\mathrm{d}x\mathrm{d}z)}{\int_{\mathcal{S}^{\mathbb{X}}} |a(x)| \xi(\mathrm{d}x)}, \quad (1)$$

$\forall \mathcal{W} \in \mathscr{X} \otimes \mathscr{Z}$, is a compatible joint of them.

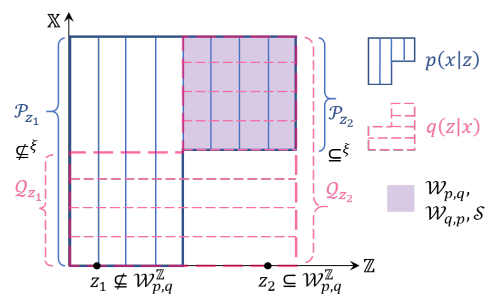

Figure 2: Illustration of our compatibility criterion in the absolutely continuous case (Thm. 2.3). The conditionals are uniform on the respective depicted slices. For condition **(i)**, $\mathcal{P}_z \subseteq^\xi \mathcal{Q}_z$ is *not* satisfied on the left half, *e.g.* z_1, so $\mathcal{W}_{p,q}$ does not cover the left half; it is satisfied on the right half, *e.g.* z_2, so $\mathcal{W}_{p,q}$ is composed of slices $\mathcal{P}_z$ on the right half, making the top-right quadrant (shaded). Similarly, $\mathcal{W}_{q,p}$ is the same region, and it is a $\xi \otimes \zeta$-complete component of itself. It also satisfies other conditions thus is a complete support $\mathcal{S}$.

Fig. 2 shows an illustration of the conditions. To understand the criterion, conditions **(iv)** and **(v)** stem from the starting inspiration, which also shows a hint for Eq. (1). Other conditions handle the subtlety to find a region $\mathcal{S}$ where **(iv)** and **(v)** must hold. This is essentially the support of a compatible joint π as there is no need and no way to control conditionals outside the support.

[4] The flexibility of $p(x|z)$ on a ξ-measure-zero set for a given z (similarly for $q(z|x)$) is not a vital problem, as one can adjust the conditions to hold only a.e.

[5] While the typical definition of support requires a topological structure which is absent under our generality, Def. B.8 in Appx. B.1 defines such a concept for absolutely continuous distributions.

[6] Formally, there exist functions a on $\mathcal{S}^{\mathbb{X}}$ and b on $\mathcal{S}^{\mathbb{Z}}$ s.t. $(\xi \otimes \zeta)\{(x, z) \in \mathcal{S} \mid \frac{p(x|z)}{q(z|x)} \neq a(x)b(z)\} = 0$.

For necessity, informally, if z is in the support of $\pi^{\mathbb{Z}}$, then $p(x|z)$ determines the distribution on $\mathbb{X}\times\{z\}$; particularly, the joint π should be a.e. positive on $\mathcal{P}_z$, which in turn asks $q(z|x)$ to be so. This means $\mathcal{P}_z \subseteq^{\xi} \mathcal{Q}_z$ (unnecessary equal, since $q(z|x)$ is "out of control" outside the joint support), which leads to the definitions of $\mathcal{W}_{p,q}$ and $\mathcal{W}_{q,p}$. The joint support should be contained within the two sets in order to avoid *support conflict* (*e.g.*, although the bottom-left quadrant in Fig. 2 is part of the intersection of positive regions of the conditionals, a joint on it is required by $p(x|z)$ to also cover the top-left, on which $q(z|x)$ does not agree). Condition **(i)** indicates $\mathcal{S} \subseteq^{\xi\otimes\zeta} \mathcal{W}_{p,q}$ and $\mathcal{W}_{q,p}$ so $\mathcal{S}$ satisfies this requirement and also makes the ratio in **(iv)** a.e. well-defined. The complete-component condition in **(i)** also makes the conditionals *normalized* on $\mathcal{S}$: as mentioned, such an $\mathcal{S}$ has a.s. the same slice as $\mathcal{W}_{p,q}$ does for a given z in support $\mathcal{S}^{\mathbb{Z}}$, so the integral of $p(x|z)$ on $\mathcal{S}_z$ is the same as that on $(\mathcal{W}_{p,q})_z$ which is 1 by construction (similarly for $q(z|x)$). Appx. Example C.3 shows $\mathcal{W}_{p,q} \cap \mathcal{W}_{q,p}$ is unnecessarily appropriate. Conditions **(ii)** and **(iii)** cannot be guaranteed by condition **(i)** (Appx. Example B.13), while are needed to rule out special cases (Appx. Lem. B.14, Example B.15). Appx. C.2 gives a rigorous proof following this intuition. Although the criterion relies on the *existence* of such a complete support, candidates are few (if any), so it is *operable*.

2.1.2 Determinacy in the absolutely continuous case

When compatible, absolutely continuous cyclic conditionals are very likely to have determinacy.

Theorem 2.4 (determinacy, absolutely continuous)**.** *Let $p(x|z)$ and $q(z|x)$ be two compatible conditional densities and $\mathcal{S}$ be a complete support that makes them compatible (also necessary due to Thm. 2.3). Suppose that $\mathcal{S}_z \overset{\xi}{=} \mathcal{S}^{\mathbb{X}}$, for ζ-a.e. z on $\mathcal{S}^{\mathbb{Z}}$, or $\mathcal{S}_x \overset{\zeta}{=} \mathcal{S}^{\mathbb{Z}}$, for ξ-a.e. x on $\mathcal{S}^{\mathbb{X}}$. Then their compatible joint supported on $\mathcal{S}$ is unique, which is given by Eq.* (1)*.*

Proof is given in Appx. C.4. The condition in the theorem roughly means that the complete support $\mathcal{S}$ is "rectangular". From the perspective of Markov chain, this corresponds to the irreducibility of the Gibbs chain ($z_1 \sim q(z|x_0), x_1 \sim p(x|z_1), \dots$) for the unique existence of a stationary distribution. When the conditionals have multiple such complete supports, on each of which the compatible joint is unique, while globally on $\mathbb{X}\times\mathbb{Z}$, they may have multiple compatible joints. In general, determinacy in the absolutely continuous case is sufficient, including the following common case (*e.g.*, in VAEs).

Corollary 2.5. *We call two conditional densities* have a.e.-full supports*, if $p(x|z) > 0, q(z|x) > 0$ for $\xi\otimes\zeta$-a.e. (x, z). If they are compatible, then their compatible joint is unique, since $\mathbb{X}\times\mathbb{Z}$ is the $\xi\otimes\zeta$-unique complete support (Prop. C.4 in Appx. C.3), which satisfies the condition in Thm. 2.4.*

2.2 Dirac Case

Many other prevailing generative models, including generative adversarial networks (GANs) [21] and flow-based models [16, 44, 32, 22], use a deterministic function $x = f(z)$ as the likelihood model. In such cases, the conditional $\mu(\mathcal{X}|z) = \delta_{f(z)}(\mathcal{X}) := \mathbb{I}[f(z) \in \mathcal{X}], \forall \mathcal{X} \in \mathscr{X}$ is a Dirac measure. Note it may not have a density function *e.g.* when ξ assigns zero to all single-point sets, like the Lebesgue measure on Euclidean spaces, so we keep the measure notion. This case is not exclusive to the absolutely continuous case: a Dirac conditional on a discrete space is also absolutely continuous.

2.2.1 Compatibility criterion in the Dirac case

Compatibility criterion is easier to imagine in this case. As illustrated in Fig. 3, it is roughly that the other-way conditional $\nu(\cdot|x)$ could find a way to put its mass only on the curve; otherwise support conflict is rendered.

Theorem 2.6 (compatibility criterion, Dirac)**.** *Suppose that $\mathscr{X}$ contains every single-point set: $\{x\} \in \mathscr{X}, \forall x \in \mathbb{X}$. Conditional distribution $\nu(\mathcal{Z}|x)$ is compatible with $\mu(\mathcal{X}|z) := \delta_{f(z)}(\mathcal{X})$ where function $f : \mathbb{Z} \to \mathbb{X}$ is $\mathscr{X}/\mathscr{Z}$-measurable*[7]*, if and only if there exists $x_0 \in \mathbb{X}$ such that $\nu(f^{-1}(\{x_0\})|x_0) = 1$.*

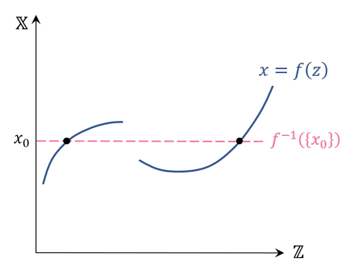

Figure 3: Illustration of our compatibility criterion in the Dirac case (Thm. 2.6).

Proof is given in Appx. C.6. Note that since the empty set always gets measure zero, such an x_0 must be in the image space $f(\mathbb{Z})$. What may be counter-intuitive is that $\nu(\cdot|x)$ is not required to concentrate on the curve for *any* x; one x_0 is sufficient as $\delta_{(x_0, f(x_0))}$ is a compatible joint. Nevertheless, in

[7] For meaningful discussion, we require f to be $\mathscr{X}/\mathscr{Z}$-measurable, which includes any function between discrete sets and continuous functions when $\mathscr{X}$ and $\mathscr{Z}$ are the Borel sigma-fields.

practice one often desires the compatibility to hold over a set $\mathcal{X}$ to be useful. When $\nu(\cdot|x)$ is also chosen to be in the Dirac form $\delta_{g(x)}$, this can be achieved by minimizing $\mathbb{E}_{p(x)}\ell\big(x, f(g(x))\big)$, where $p(x)$ is a distribution on $\mathcal{X}$ and ℓ is a metric on $\mathbb{X}$. This is the *cycle-consistency loss* used in dual learning [30, 67, 65, 41]. When f is invertible, achieving zero of this loss is also necessary, as there is only one element in $f^{-1}(x)$ for any $x \in \mathcal{X}$. So flow-based models are naturally compatible.

2.2.2 Determinacy in the Dirac case

As explained above, for any x_0 satisfying the condition, the two conditionals have determinacy on this point $\{x_0\}$ with compatible joint $\delta_{(x_0, f(x_0))}$. Similar to the absolutely continuous case, when such x_0 is not unique, there are multiple compatible joints globally on $\mathbb{X}\times\mathbb{Z}$. This is however often the case, as compatibility is usually desired to hold on a set $\mathcal{X}$ (with multiple elements) to be useful, but a joint distribution on $\mathcal{X}$ cannot be determined uniquely. This meets one's intuition: compatible Dirac conditionals can only determine a curve in $\mathbb{X}\times\mathbb{Z}$ from two sides, but the distribution on the curve is undetermined. One exception is when $f(z) \equiv x_0$ is constant, so this x_0 is the only candidate in the theorem. The joint then degenerates to a distribution on $\mathbb{Z}$, which is fully determined by $\nu(\cdot|x_0)$.

In general, determinacy in the Dirac case is insufficient, and this type of generative models (GANs, flow-based models) have to specify a prior to define a joint.

3 Generative Modeling using Cyclic Conditionals

The theory suggests it is possible that two conditionals achieve compatibility and particularly a sufficient determinacy, so that they can define a useful joint distribution without specifying a prior for generative modeling. For a sufficient determinacy, a deterministic likelihood or inference model is undesired due to the analysis on the Dirac case, so we consider absolutely continuous conditionals and use probabilistic likelihood and inference models, represented by parameterized density models $p_\theta(x|z)$, $q_\phi(z|x)$. Note that given determinacy, a certain prior is implicitly determined, and the following methods do not require an explicit model for this prior. We take $\mathbb{X}$, $\mathbb{Z}$ as Euclidean spaces $\mathbb{R}^{d_\mathbb{X}}$, $\mathbb{R}^{d_\mathbb{Z}}$, which is common in generative modeling, and assume the conditional densities have a.e.-full supports and are differentiable, which hold for common architectures.

As a generative model, the conditionals are first expected to be compatible as the prerequisite for determinacy. They then need to fit their determined distribution $p_{\theta,\phi}(x)$ to the data distribution $p^*(x)$. After learning, they are also expected to generate novel data samples. We now develop methods for the three tasks, and call the resulting framework CyGen for "**Cy**clic **Gen**erative" modeling.

3.1 Enforcing Compatibility

In the a.e.-full support case, the entire space $\mathbb{X}\times\mathbb{Z}$ is the only possible complete support (Prop. C.4 in Appx. C.3), so for compatibility, condition **(iv)** in Thm. 2.3 is the most critical one. For this, we do not have to find functions $a(x)$, $b(z)$ in Thm. 2.3, but only need to enforce such a factorization. So we propose the following loss function to enforce compatibility:

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

Here, ρ is some absolutely continuous reference distribution on $\mathbb{X}\times\mathbb{Z}$, which can be taken as $p^*(x)q_\phi(z|x)$ in practice as it gives samples to estimate the expectation. When $C(\theta,\phi) = 0$, we have $\nabla_x\nabla_z^\top r_{\theta,\phi}(x,z) = 0$, $\xi\otimes\zeta$-a.e. [9, Thm. 15.2(ii)]. By integration, this means $\nabla_z r_{\theta,\phi}(x,z) = V(z)$ hence $r_{\theta,\phi}(x,z) = v(z) + u(x)$, $\xi\otimes\zeta$-a.e., for some functions $V(z)$, $v(z)$, $u(x)$ such that $V(z) = \nabla v(z)$. So the ratio $p_\theta(x|z)/q_\phi(z|x) = \exp\{r_{\theta,\phi}(x,z)\} = \exp\{u(x)\}\exp\{v(z)\}$ factorizes, $\xi\otimes\zeta$-a.s. This compatibility loss is different from the Jacobian norm regularizers of contractive AE [51] and DAE [51, 1], and explains the successful tied weights trick [61, 51, 1] (see Appx. D.1).

Implication on Gaussian VAE which uses additive Gaussian conditional models, $p_\theta(x|z) := \mathcal{N}(x|f_\theta(z), \sigma_d^2 I_{d_\mathbb{X}})$ and $q_\phi(z|x) := \mathcal{N}(z|g_\phi(x), \sigma_e^2 I_{d_\mathbb{Z}})$. It is the vanilla and the most common form of VAE [33]. As its ELBO objective drives $q_\phi(z|x)$ to meet the joint $p(z)p_\theta(x|z)$, compatibility is enforced. Under our view, this amounts to minimizing the compatibility loss Eq. (2), which then enforces the match of Jacobians: $(\nabla_z f_\theta^\top(z))^\top = (\sigma_d^2/\sigma_e^2)\nabla_x g_\phi^\top(x)$. As the two sides indicate the equation is constant of both x and z, it must be a constant, so $f_\theta(z)$ *and* $g_\phi(x)$ *must be affine*. This conclusion coincides with the theory on additive noise models [66, 46], and explains the empirical observation that the latent space of such VAEs is quite linear [55]. It is also the root of recent analyses on Gaussian VAE that the latent space coordinates the data manifold [14] and the encoder learns an isometric embedding after a proper rescaling [42].

This finding reveals that the expectation to use deep neural networks for learning a flexible nonlinear representation will be disappointed in Gaussian VAE. So we use a non-additive-Gaussian model, *e.g.* a flow-based model [49, 34, 59, 22], for at least one of $p_\theta(x|z)$ and $q_\phi(z|x)$ (often the latter).

Efficient implementation. Direct Jacobian evaluation for Eq. (2) is of complexity $O(d_{\mathbb{X}} d_{\mathbb{Z}})$, which is often prohibitively large. We thus propose a stochastic but much cheaper and unbiased method based on Hutchinson's trace estimator [28]: $\mathrm{tr}(A) = \mathbb{E}_{p(\eta)}[\eta^\top A \eta]$, where η is any random vector with zero mean and identity covariance (*e.g.*, a standard Gaussian). As the function within expectation is $\left\|\nabla_x \nabla_z^\top r\right\|_F^2 = \left\|\nabla_z \nabla_x^\top r\right\|_F^2 = \mathrm{tr}\left((\nabla_z \nabla_x^\top r)^\top \nabla_z \nabla_x^\top r\right)$, applying the estimator yields a formulation that reduces gradient evaluation complexity to $O(d_{\mathbb{X}} + d_{\mathbb{Z}})$:

$$(\min_{\theta,\phi}) \;\; C(\theta,\phi) = \mathbb{E}_{\rho(x,z)} \mathbb{E}_{p(\eta_x)} \left\| \nabla_z \left(\eta_x^\top \nabla_x r_{\theta,\phi}(x,z) \right) \right\|_2^2, \text{where } \mathbb{E}[\eta_x] = 0, \mathrm{Var}[\eta_x] = I_{d_{\mathbb{X}}}. \quad (3)$$

As concluded from the above analysis on Gaussian VAE, we use a flow-based model for the inference model $q_\phi(z|x)$. But in common instances evaluating the inverse of the flow is intractable [49, 34, 59] or costly [22]. This however, disables the use of automatic differentiation tools for estimating the gradients in the compatibility loss. Appx. D.2 explains this problem in detail and shows our solution.

3.2 Fitting Data

In the a.e.-full support case, compatible conditionals enjoy a quite sufficient determinacy that the compatible joint is unique on $\mathbb{X} \times \mathbb{Z}$ (Cor. 2.5). To fit data distribution $p^*(x)$, an explicit expression of the model-determined distribution $p_{\theta,\phi}(x)$ is required. For this, Eq. (1) is not very helpful as we do not have explicit expressions of $a(x)$, $b(z)$ in Thm. 2.3. But when compatibility is given, we can safely use density-function calculus for deduction:

$$p_{\theta,\phi}(x) = 1 \Big/ \tfrac{1}{p_{\theta,\phi}(x)} = 1 \Big/ \int_{\mathbb{Z}} \tfrac{p_{\theta,\phi}(z')}{p_{\theta,\phi}(x)} \zeta(\mathrm{d}z') = 1 \Big/ \int_{\mathbb{Z}} \tfrac{q_\phi(z'|x)}{p_\theta(x|z')} \zeta(\mathrm{d}z') = 1 / \mathbb{E}_{q_\phi(z'|x)}[1/p_\theta(x|z')],$$

which is an explicit expression in terms of the two conditionals. Although other expressions are possible, this one has a simple form, and the Monte-Carlo expectation estimation in $\mathbb{Z}$ has a lower variance than in $\mathbb{X}$ as usually $d_{\mathbb{Z}} \ll d_{\mathbb{X}}$. We can thus fit data by maximum likelihood estimation:

$$(\min_{\theta,\phi}) \;\; \mathbb{E}_{p^*(x)}[-\log p_{\theta,\phi}(x)] = \mathbb{E}_{p^*(x)}[\log \mathbb{E}_{q_\phi(z'|x)}[1/p_\theta(x|z')]]. \quad (4)$$

The loss function can be estimated using the reparameterization trick [33] to reduce variance, and the `logsumexp` trick is adopted for numerical stability. This expression can also serve for data likelihood evaluation. The final training process of CyGen is the joint optimization with the compatibility loss.

Comparison with DAE. We note that the DAE loss [61, 6] $\mathbb{E}_{p^*(x)q_\phi(z'|x)}[-\log p_\theta(x|z')]$ is a *lower bound* of this loss Eq. (4) due to Jensen's inequality. So minimizing the DAE loss may not lead to a maximum likelihood estimate. In fact, the DAE loss minimizes $\mathbb{E}_{q_\phi(z)} \mathrm{KL}(q_\phi(x|z) \| p_\theta(x|z))$ for $p_\theta(x|z)$ to match $q_\phi(x|z)$, where $q_\phi(z)$ and $q_\phi(x|z)$ are induced from the joint $p^*(x)q_\phi(z|x)$, but it is not a proper loss for $q_\phi(z|x)$ as a mode-collapse behavior is promoted: an optimal $q_\phi(z|x)$ only concentrates on points in $\mathrm{argmin}_{z'} p_\theta(x|z')$ for every x in the support of $p^*(x)$, and an additional entropy term $-\mathbb{E}_{q_\phi(z)} \mathbb{H}[q_\phi(x|z)]$ is required to optimize the same KL loss. This hurts determinacy, as $q_\phi(z|x)$ tends to be a (mixture of) Dirac measure (Sec. 2.2.2), and the resulting Gibbs chain may have multiple stationary distributions depending on initialization (as ergodicity is broken). This tendency of $q_\phi(z|x)$ also deviates $q_\phi(x|z)$ from $p_\theta(x|z)$, which hurts compatibility, so $q_\phi(z|x)$ is then not the conditional of a Gibbs stationary distribution [6]. In contrast, CyGen follows a more fundamental logic: explicitly enforce compatibility and faithfully follow the maximum likelihood principle, leading to a proper loss for both conditionals that does not hinder determinacy.

3.3 Data Generation

Generating novel data samples from $p_{\theta,\phi}(x)$ determined by the two conditionals $p_\theta(x|z)$ and $q_\phi(z|x)$ is not as straightforward as the typical prior-likelihood generative models. But it is still practical.

Gibbs sampling has been considered [6, 38] to draw samples from a joint distribution represented by two conditionals. The sampling procedure is to alternately draw from $p_\theta(x|z)$ and $q_\phi(z|x)$, *i.e.*, $z_t \sim q_\phi(z|x_{t-1})$, $x_t \sim p_\theta(x|z_t)$, $t = 1, 2, \cdots$. In the a.e.-full support case, the chain has a unique stationary distribution since ergodicity is satisfied, and given compatibility, this is exactly the joint that they determine. Gibbs sampling is easy to implement, but often converges insufficiently fast.

Dynamics-based MCMCs are often more efficient, due to the leverage of gradient information. Generating samples from the marginal distribution $p_{\theta,\phi}(x)$ only requires an unnormalized density function of $p_{\theta,\phi}(x)$ for which CyGen could well serve when compatible: $p_{\theta,\phi}(x) = \frac{p_{\theta,\phi}(x)}{p_{\theta,\phi}(z)} p_{\theta,\phi}(z) = \frac{p_\theta(x|z)}{q_\phi(z|x)} p_{\theta,\phi}(z) \propto \frac{p_\theta(x|z)}{q_\phi(z|x)}, \forall z \in \mathbb{Z}$. In practice, this z can be taken as a sample from $q_\phi(z|x)$ to lie in a high probability region for a more confident estimate. For a representative method, stochastic gradient Langevin dynamics (SGLD) [62] gives the following transition:

$$x^{(t+1)} = x^{(t)} + \varepsilon \nabla_{x^{(t)}} \log \frac{p_\theta(x^{(t)}|z^{(t)})}{q_\phi(z^{(t)}|x^{(t)})} + \sqrt{2\varepsilon}\eta_x^{(t)}, \text{where } z^{(t)} \sim q_\phi(z|x^{(t)}), \eta_x^{(t)} \sim \mathcal{N}(0, I_{d_{\mathbb{X}}}), \quad (5)$$

and ε is a step size parameter. Method to draw from the prior $p_{\theta,\phi}(z)$ can be developed symmetrically.

4 Experiments

We demonstrate the power of CyGen on a variety of generation and inference tasks on synthetic and real-world datasets. Data generation and representation learning performances are compared against other bi-directional generative models using a specified standard Gaussian prior, including VAE and BiGAN (see Appx. E.1).

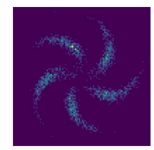

Figure 4: Synthetic data distribution.

4.1 Synthetic Experiments

For easy visual verification of the claims, we first consider a 2D toy dataset illustrated in Fig. 4, in the form of the histogram of data samples. All methods share the same architecture of an additive Gaussian $p_\theta(x|z)$ and a Sylvester flow [59] $q_\phi(z|x)$. Appx. E.2, E.3 show more details and results.

Data generation. The learned data distributions (as histogram of generated data) and aggregated posteriors (as scatter plot of z samples from $q_\phi(z|x)p^*(x)$) are visualized in Table 1. We see that VAE generates a blurry data distribution and the generated components of BiGAN are still connected. The specified prior with a connected support makes it hard to fit this distribution whose support is nearly non-connected. In contrast, our CyGen better fits this distribution; particularly it shows a clearer boundary of each component. This verifies the advantage of overcoming the *manifold mismatch* problem.

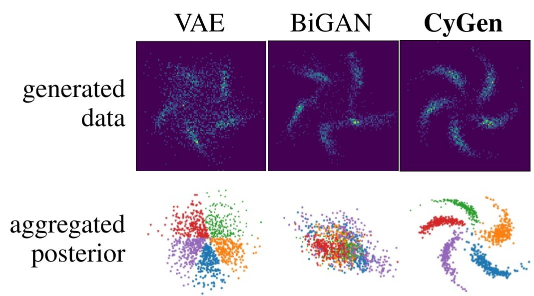

Table 1: Generated data (SGLD for CyGen) and aggregated posterior of VAE, BiGAN and CyGen.

Inference. Results of the aggregated posterior in Table 1 (row 2) show that CyGen mitigates the *posterior collapse* problem, as the learned inference model $q(z|x)$ better separates data clusters in the latent space. This more informative and representative latent code would make a better performance on downstream tasks like classification or clustering on the latent space. In contrast, the specified unimodal prior squeezes the VAE latent clusters to touch, and the BiGAN latent clusters even to mix.

Comparison of data generation methods for CyGen. We then make more analysis on CyGen. Table 2 (rows 1,2) shows generated data of CyGen using SGLD and Gibbs sampling (100 transition steps for both). We see SGLD better recovers the true distribution, and is more robust to slight incompatibility, due to the leverage of gradient information and the resulting faster mixing of the chain.

Impact of the compatibility loss. Table 2 (rows 1,3) also shows the comparison with training CyGen without the compatibility loss. We see the compatibility is indeed out of control without the loss, which

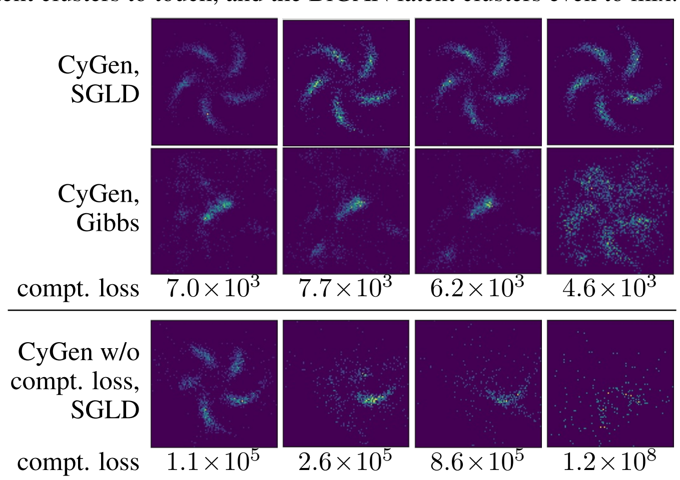

Table 2: Generated data using SGLD and Gibbs sampling along the training process of CyGen w/ and w/o the compatibility loss (initialized by a pretrained VAE). See also Appx. Table 5.

then invalidates the likelihood estimation Eq. (4) for fitting data and the gradient estimation in Eq. (5) for data generation, leading to the failure in row 3. Along the training process of the normal CyGen, we also find a smaller compatibility loss makes better generation (esp. using Gibbs sampling).

Incorporating knowledge into the conditionals. Appx. Fig. 11 shows CyGen successfully learns a centered and centrosymmetic prior when using the likelihood model of a VAE with prior $\mathcal{N}(0, I)$.

4.2 Real-World Datasets

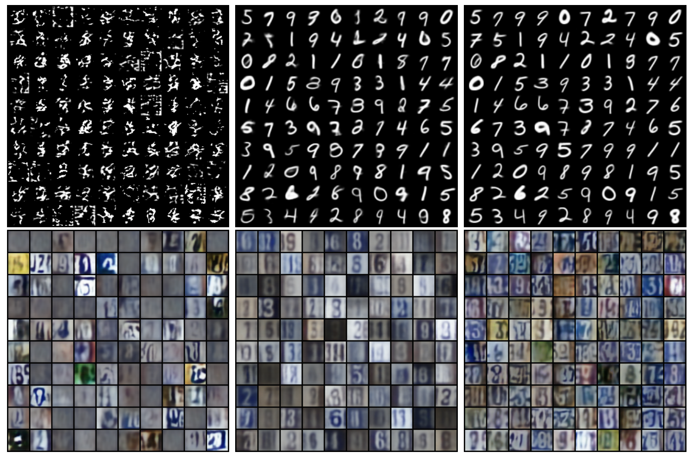

Figure 5: Generated samples on MNIST/SVHN dataset by DAE (left), VAE (middle), and **CyGen** by SGLD (right).

We test the performance of CyGen on real-world image datasets MNIST and SVHN against VAE and DAE using the same model architecture. From the analysis on Gaussian VAE in Sec. 3.1, we use the Sylvester flow (Householder version) [59] to implement the inference model. For stable training and incorporating certain knowledge, CyGen is initialized by a pretrained VAE. CyGen generates data by SGLD from $x_0 \sim q_\phi(\cdot|z_0)$ where $z_0 \sim \mathcal{N}(0, I)$, and DAE by its standard Gibbs sampling procedure from such a z_0. We also tried BiGAN and GibbsNet, but did not see reasonable results with our model architecture, possibly due to the even more unstable mini-max optimization in this case with stochastic conditionals and involved gradient back-propagation. Appx. E.4 shows more details.

Data generation. Generated samples of these methods are shown in Fig. 5. We see that CyGen generates both sharp and diverse samples. Samples by DAE are mostly imperceptible, due to the mode-collapse behavior of $q_\phi(z|x)$ and the subsequent lack of compatibility and determinacy (Sec. 3.2) and the difficulty to capture the data distribution. VAE generates a little blurry samples, as is its typical behavior due to the simply-connected prior.

Table 3: Downstream classification accuracy (%) using learned representation by various generative models. BiGAN and GibbsNet results are from [38] with a different, deterministic architecture (not suitable for determinacy). They make random guess using the flow architecture.

	VAE	DAE	BiGAN	GibbsNet	**CyGen**
MNIST	$94.5_{\pm 0.3}$	$98.0_{\pm 0.1}$	91.0	97.7	$\mathbf{98.3}_{\pm 0.1}$
SVHN	$30.8_{\pm 0.2}$	$74.5_{\pm 1.0}$	67.7	**77.0**	$\mathbf{75.8}_{\pm 0.5}$

Inference. We then show in Table 3 that the latent representation learned by CyGen is more informative for the downstream classification task, as an indicator to avoid posterior collapse. BiGAN and GibbsNet make random guess using our flow architecture due to the mentioned instability, so we only show the reported results in [38] that use a different, deterministic architecture (which is not suitable for CyGen due to insufficient determinacy). The results show that by removing the prior constraint and using a more reasonable loss using CyGen, the stochastic representation preserves more information of data than using VAE and DAE, and is comparable or better than deterministic representations using BiGAN and GibbsNet. We conclude that CyGen achieves both superior generation and representation learning performances.

5 Conclusions

In this work we investigate the possibility of defining a joint distribution using two conditionals under the consideration for generative modeling without an explicit prior distribution. We develop a systematic theory with novel and operable equivalence criteria for compatibility and sufficient conditions for determinacy, and exploit the theory to develop practical methods for generative modeling using cyclic conditionals (*i.e.*, CyGen), including enforcing compatibility, fitting data and data generation. Experiments show the benefits of CyGen over generative models with specified prior and DAE-like models in overcoming the manifold mismatch and posterior collapse problems.

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Supplementary Materials

A Background in Measure Theory

A.1 The Integral

The *integral* of a nonnegative measurable function f on a measure space $(\Omega, \mathscr{F}, \mu)$ is defined as:

$$\int f \,\mathrm{d}\mu := \sup \sum_i \mu(\mathcal{W}^{(i)}) \inf_{\omega \in \mathcal{W}^{(i)}} f(\omega),$$

where the supremum is taken over all finite decompositions $\{\mathcal{W}^{(i)}\}$ of Ω into $\mathscr{F}$-sets [9, p.211]. For a general measurable function, its integral is defined as the subtraction from the integral of its positive part $f^+(\omega) := \max\{0, f(\omega)\}$ with the integral of its negative part $f^-(\omega) := \max\{0, -f(\omega)\}$. A measurable function is said to be *μ-integrable* [9, p.212] if both integrals of its positive and negative parts are finite.

(i) This is a general definition of integral. When Ω is an Euclidean space and μ is the Lebesgue measure on it, this integral reduces to the Lebesgue integral (which in turn coincides with the Riemann integral when the latter exists). When Ω is a discrete set (*i.e.*, a finite or countable set) and μ is the counting measure, this integral reduces to summation.

(ii) The integral satisfies common properties like linearity and monotonicity [9, Thm. 16.1], continuity under boundedness [9, Thm. 16.4, Thm. 16.5], *etc.* For a nonnegative function f, $\int f \,\mathrm{d}\mu = 0$ if and only if $f = 0$, μ-a.e. [9, Thm. 15.2].

(iii) The integral over a set $\mathcal{W} \in \mathscr{F}$ is defined as $\int_{\mathcal{W}} f \,\mathrm{d}\mu := \int \mathbb{I}_{\mathcal{W}} f \,\mathrm{d}\mu$ [9, p.226], where $\mathbb{I}_{\mathcal{W}}$ is the indicator function.
(1) We thus sometimes also write $\int_{\Omega} f \,\mathrm{d}\mu$ for $\int f \,\mathrm{d}\mu$ to highlight the integral area. By this definition, $\int_{\mathcal{W}} f \,\mathrm{d}\mu = 0$ if $\mu(\mathcal{W}) = 0$ [9, p.226].
(2) For two measurable functions f and g, if $f = g$, μ-a.e., then $\int_{\mathcal{W}} f \,\mathrm{d}\mu = \int_{\mathcal{W}} g \,\mathrm{d}\mu$ for any $\mathcal{W} \in \mathscr{F}$ [9, Thm. 15.2]. The inverse also holds if f and g are nonnegative and μ is sigma-finite, or f and g are integrable [9, Thm. 16.10(i,ii)][8].
(3) If f is a nonnegative measurable function, then $\nu(\mathcal{W}) := \int_{\mathcal{W}} f \,\mathrm{d}\mu$, $\forall \mathcal{W} \in \mathscr{F}$, is a measure on $(\Omega, \mathscr{F})$ [9, p.227][9]. Such a measure ν is finite, if and only if f is μ-integrable.

A.2 Absolute Continuity and Radon-Nikodym Derivative

For two measures μ and ν on the same measurable space $(\Omega, \mathscr{F})$, ν is said to be *absolutely continuous* w.r.t μ, denoted as $\nu \ll \mu$, if $\mu(\mathcal{W}) = 0$ indicates $\nu(\mathcal{W}) = 0$ for $\mathcal{W} \in \mathscr{F}$ [9, p.448]. If μ and ν are sigma-finite and $\nu \ll \mu$, the *Radon-Nikodym theorem* [9, Thm. 32.2] asserts that there exists a μ-unique nonnegative function f on Ω, such that $\nu(\mathcal{W}) = \int_{\mathcal{W}} f(\omega)\mu(\mathrm{d}\omega)$ for any $\mathcal{W} \in \mathscr{F}$. Such a function f is called the *Radon-Nikodym (R-N) derivative* of ν w.r.t μ, and is also denoted as $\frac{\mathrm{d}\nu}{\mathrm{d}\mu}$. It represents the density function of ν w.r.t base measure μ.

(i) Since the general definition of integral includes summation in the discrete case, this density function also includes the probability mass function in the discrete case.

(ii) The Dirac measure $\delta_{\omega_0}(\mathcal{W}) := \mathbb{I}_{\mathcal{W}}(\omega_0)$ ($\mathbb{I}$ is the indicator function) at a single point $\omega_0 \in \Omega$ is not absolutely continuous on Euclidean spaces w.r.t the Lebesgue measure, which assigns measure 0 to the set $\{\omega_0\}$. To be strict, the Dirac delta function is not a proper density function, since its integrals covering ω_0 involve the indefinite $\infty \cdot 0$ on the component $\{\omega_0\}$ of the integral domain. Its characteristic that such integrals equal to one, is a standalone structure from being a function. So it is better treated as a measure of functional.

A.3 Product Measure Space

Two measure spaces $(\mathbb{X}, \mathscr{X}, \xi)$ and $(\mathbb{Z}, \mathscr{Z}, \zeta)$ induce a *product measure space* $(\mathbb{X} \times \mathbb{Z}, \mathscr{X} \otimes \mathscr{Z}, \xi \otimes \zeta)$.

[8] 9, Thm. 16.10(iii): $f = g$, μ-a.e., if $\int_{\mathcal{W}} f \,\mathrm{d}\mu = \int_{\mathcal{W}} g \,\mathrm{d}\mu$ for any $\mathcal{W}$ from a pi-system Π that generates $\mathscr{F}$, and Ω is a finite or countable union of Π-sets.

[9] Its countable additivity is guaranteed by Billingsley [9, Thm. 16.9].

(i) The *product sigma-field* $\mathscr{X} \otimes \mathscr{Z} := \sigma(\mathscr{X} \times \mathscr{Z})$ is the smallest sigma-field on $\mathbb{X}\times\mathbb{Z}$ containing $\mathscr{X} \times \mathscr{Z}$ (20, Thm. 22; 53, Def. 7.1; equivalently, 35, Remark 14.10; 35, Def. 14.4). Note that the Cartesian product $\mathscr{X} \times \mathscr{Z}$, representing the set of *measurable rectangles*, is only a semiring (thus also a pi-system). So we need to extend for a sigma-field. For any $\mathcal{W} \in \mathscr{X} \otimes \mathscr{Z}$, its *slice* (or section) at $z \in \mathbb{Z}$, defined by:

$$\mathcal{W}_z := \{x \mid (x, z) \in \mathcal{W}\},$$

lies in $\mathscr{X}$, and similarly $\mathcal{W}_x \in \mathscr{Z}$ [9, Thm. 18.1(i)]. We define the *projection* (or restriction) of $\mathcal{W}$ onto $\mathbb{Z}$, as $\mathcal{W}^{\mathbb{Z}} := \{z \mid \exists x \in \mathbb{X} \text{ s.t. } (x, z) \in \mathcal{W}\}$. By definition, for any $z \in \mathbb{Z} \setminus \mathcal{W}^{\mathbb{Z}}$, $\mathcal{W}_z = \emptyset$.

(ii) The *product measure* $\xi\otimes\zeta$ is characterized by $(\xi\otimes\zeta)(\mathcal{X}\times\mathcal{Z}) = \xi(\mathcal{X})\zeta(\mathcal{Z})$ for measurable rectangles $\mathcal{X}\times\mathcal{Z} \in \mathscr{X} \times \mathscr{Z}$. Some common conclusions require ξ and ζ to be sigma-finite on $\mathscr{X}$ and $\mathscr{Z}$, respectively.
(1) In the characterization $(\xi\otimes\zeta)(\mathcal{X}\times\mathcal{Z}) = \xi(\mathcal{X})\zeta(\mathcal{Z})$, if the indefinite $0 \cdot \infty$ is met, it is zero. To see this, consider two sets $\mathcal{X}$ and $\mathcal{Z}$ that satisfy $\xi(\mathcal{X}) = 0$ and $\zeta(\mathcal{Z}) = 0$. Since ζ is sigma-finite, there are finite or countable disjoint $\mathscr{Z}$-sets $\mathcal{Z}^{(1)}, \mathcal{Z}^{(2)}, \cdots$ such that $\zeta(\mathcal{Z}^{(i)}) < \infty$ for any $i \geqslant 1$ and $\bigcup_{i=1}^{\infty} \mathcal{Z}^{(i)} = \mathbb{Z}$. Redefining $\mathcal{Z}^{(i)}$ as $\mathcal{Z}^{(i)} \cap \mathcal{Z}$, we have $\bigcup_{i=1}^{\infty} \mathcal{Z}^{(i)} = \mathcal{Z}$ while still $\zeta(\mathcal{Z}^{(i)}) < \infty$. So $(\xi\otimes\zeta)(\mathcal{X}\times\mathbb{Z}) = (\xi\otimes\zeta)(\mathcal{X}\times\bigcup_{i=1}^{\infty} \mathcal{Z}^{(i)}) = (\xi\otimes\zeta)(\bigcup_{i=1}^{\infty} \mathcal{X}\times\mathcal{Z}^{(i)})$. Recalling that a measure is countably additive by definition, this is $= \sum_{i=1}^{\infty}(\xi\otimes\zeta)(\mathcal{X}\times\mathcal{Z}^{(i)}) = \sum_{i=1}^{\infty}\xi(\mathcal{X})\zeta(\mathcal{Z}^{(i)}) = 0$.
(2) In this case, such a $\xi\otimes\zeta$ is sigma-finite on $\mathscr{X} \times \mathscr{Z}$, and the characterization on the pi-system $\mathscr{X} \times \mathscr{Z}$ determines a unique sigma-finite measure on $\sigma(\mathscr{X} \times \mathscr{Z}) = \mathscr{X} \otimes \mathscr{Z}$ [9, Thm. 10.3]. See also Galambos [20, Thm. 22]; Klenke [35, Thm. 14.14]; Rinaldo [53, Thm. 7.9]. Moreover, we have [9, Thm. 18.2]:

$$(\xi\otimes\zeta)(\mathcal{W}) = \int_{\mathbb{Z}} \xi(\mathcal{W}_z)\zeta(\mathrm{d}z) = \int_{\mathbb{X}} \zeta(\mathcal{W}_x)\xi(\mathrm{d}x),\ \forall\mathcal{W} \in \mathscr{X} \otimes \mathscr{Z}. \tag{6}$$

Since for any $z \in \mathbb{Z} \setminus \mathcal{W}^{\mathbb{Z}}$, $\mathcal{W}_z = \emptyset$ (see **(i)**) thus $\xi(\mathcal{W}_z) = 0$, we also have (by leveraging the additivity of integrals over a countable partition [9, Thm. 16.9] and that an a.e. zero function gives a zero integral [9, Thm. 15.2(i)]):

$$(\xi\otimes\zeta)(\mathcal{W}) = \int_{\mathcal{W}^{\mathbb{Z}}} \xi(\mathcal{W}_z)\zeta(\mathrm{d}z) = \int_{\mathcal{W}^{\mathbb{X}}} \zeta(\mathcal{W}_x)\xi(\mathrm{d}x),\ \forall\mathcal{W} \in \mathscr{X} \otimes \mathscr{Z}. \tag{7}$$

(iii) For a function f on $\mathbb{X}\times\mathbb{Z}$, if it is $\mathscr{X} \otimes \mathscr{Z}$-measurable, then $f(x, \cdot)$ is $\mathscr{Z}$-measurable for any $x \in \mathbb{X}$, and $f(\cdot, z)$ is $\mathscr{X}$-measurable for any $z \in \mathbb{Z}$ [9, Thm. 18.1(ii)]. When f is $\xi\otimes\zeta$-integrable, *Fubini's theorem* [9, Thm. 18.3] asserts its integral on $\mathbb{X}\times\mathbb{Z}$ can be computed iteratedly in either order:

$$\int_{\mathbb{X}\times\mathbb{Z}} f(x, z)(\xi\otimes\zeta)(\mathrm{d}x\mathrm{d}z) = \int_{\mathbb{Z}} \left(\int_{\mathbb{X}} f(x, z)\xi(\mathrm{d}x)\right) \zeta(\mathrm{d}z) = \int_{\mathbb{X}} \left(\int_{\mathbb{Z}} f(x, z)\zeta(\mathrm{d}z)\right) \xi(\mathrm{d}x). \tag{8}$$

For any $\mathcal{W} \in \mathscr{X} \otimes \mathscr{Z}$, the same equalities hold for function $\mathbb{I}_{\mathcal{W}} f$. For the first iterated integral, we have $\int_{\mathbb{X}} \mathbb{I}_{\mathcal{W}}(x, z)f(x, z)\xi(\mathrm{d}x) = \int_{\mathbb{X}} \mathbb{I}_{\mathcal{W}_z}(x)f(x, z)\xi(\mathrm{d}x) = \int_{\mathcal{W}_z} f(x, z)\xi(\mathrm{d}x)$, and on the region $\mathbb{Z} \setminus \mathcal{W}^{\mathbb{Z}}$, the integral $\int_{\mathcal{W}_z} f(x, z)\xi(\mathrm{d}x) = 0$ [9, p.226] since $\mathcal{W}_z = \emptyset$ on that region (see **(i)**). So we have a more general form of Fubini's theorem:

$$\int_{\mathcal{W}} f(x, z)(\xi\otimes\zeta)(\mathrm{d}x\mathrm{d}z) = \int_{\mathcal{W}^{\mathbb{Z}}} \left(\int_{\mathcal{W}_z} f(x, z)\xi(\mathrm{d}x)\right) \zeta(\mathrm{d}z) = \int_{\mathcal{W}^{\mathbb{X}}} \left(\int_{\mathcal{W}_x} f(x, z)\zeta(\mathrm{d}z)\right) \xi(\mathrm{d}x). \tag{9}$$

(iv) For a measure π on the product measurable space $(\mathbb{X}\times\mathbb{Z}, \mathscr{X}\otimes\mathscr{Z})$, define its marginal distributions: $\pi^{\mathbb{X}}(\mathcal{X}) := \pi(\mathcal{X}\times\mathbb{Z}), \forall\mathcal{X} \in \mathscr{X}$, and $\pi^{\mathbb{Z}}(\mathcal{Z}) := \pi(\mathbb{X}\times\mathcal{Z}), \forall\mathcal{Z} \in \mathscr{Z}$.

A.4 Conditional Distributions

In the most general case, a distribution (probability measure) π on a measurable space $(\Omega, \mathscr{F})$ gives a *conditional distribution* (conditional probability) $\pi(\mathcal{W}|\omega)$ for $\mathcal{W} \in \mathscr{F}$ w.r.t a sub-sigma-field $\mathscr{G} \subseteq \mathscr{F}$.

(i) For any $\mathcal{W} \in \mathscr{F}$, the function $\mathscr{G} \to \mathbb{R}^{\geqslant 0}, \mathcal{G} \mapsto \pi(\mathcal{G} \cap \mathcal{W})$ gives a measure on $\mathscr{G}$. It is absolutely continuous w.r.t $\pi^{\mathscr{G}} : \mathscr{G} \to \mathbb{R}^{\geqslant 0}, \mathcal{G} \mapsto \pi(\mathcal{G})$, the projection of π onto $\mathscr{G}$, due to the monotonicity (or (sub-)additivity) of measures. So the R-N derivative on $\mathscr{G}$ exists, which defines the conditional distribution [9, p.457]:

$$\pi(\mathcal{W}|\omega) := \frac{\mathrm{d}\pi(\cdot \cap \mathcal{W})}{\mathrm{d}\pi^{\mathscr{G}}(\cdot)}(\omega),$$

where $\omega \in \Omega$. Note that as defined as an R-N derivative, the conditional distribution is only $\pi^{\mathscr{G}}$-unique.

(ii) As a function of ω, $\pi(\mathcal{W}|\omega)$ is $\mathscr{G}$-measurable and π-integrable, and satisfies [9, p.457, Thm. 33.1]:

$$\int_{\mathcal{G}} \pi(\mathcal{W}|\omega)\pi^{\mathscr{G}}(\mathrm{d}\omega) = \pi(\mathcal{G} \cap \mathcal{W}), \forall \mathcal{G} \in \mathscr{G}. \tag{10}$$

This could serve as an alternative definition of conditional probability.

(iii) For $\pi^{\mathscr{G}}$-a.e. ω, $\pi(\cdot|\omega)$ is a distribution (probability measure) on $(\Omega, \mathscr{F})$ [9, Thm. 33.2].

(iv) Conditional distributions on a product measurable space $(\mathbb{X}\times\mathbb{Z}, \mathscr{X}\otimes\mathscr{Z})$. Consider the sub-sigma-field $\mathscr{G} := \{\mathbb{X}\}\times\mathscr{Z}$. By construction, any $\mathcal{G} \in \mathscr{G}$ can be formed by $\mathcal{G} = \mathbb{X}\times\mathcal{Z}$ for some $\mathcal{Z} \in \mathscr{Z}$. So $\pi^{\mathscr{G}}(\mathcal{G}) := \pi(\mathcal{G}) = \pi(\mathbb{X}\times\mathcal{Z}) =: \pi^{\mathbb{Z}}(\mathcal{Z})$, and Eq. (10) becomes $\pi\big((\mathbb{X}\times\mathcal{Z}) \cap \mathcal{W}\big) = \int_{\mathbb{X}\times\mathcal{Z}} \pi(\mathcal{W}|x,z)\pi^{\mathscr{G}}(\mathrm{d}x\mathrm{d}z) = \int_{\mathbb{X}\times\mathcal{Z}} \pi(\mathcal{W}|x,z)\pi^{\mathbb{Z}}(\mathrm{d}z) = \int_{\mathcal{Z}} \pi(\mathcal{W}|x,z)\pi^{\mathbb{Z}}(\mathrm{d}z)$. This indicates that the conditional probability $\pi(\mathcal{W}|x,z)$ in this case is constant w.r.t x. We hence denote it as $\pi(\mathcal{W}|z)$.

Consider $\mathcal{W} \in \mathscr{X}\otimes\mathscr{Z}$ in the form $\mathcal{W} = \mathcal{X}\times\mathbb{Z}$ for some $\mathcal{X} \in \mathscr{X}$. For any $\mathcal{G} = \mathbb{X}\times\mathcal{Z} \in \mathscr{G}$, we have from Eq. (10) that $\int_{\mathcal{G}} \pi(\mathcal{W}|z)\pi^{\mathscr{G}}(\mathrm{d}x\mathrm{d}z) = \pi(\mathcal{G} \cap \mathcal{W}) = \pi(\mathcal{X}\times\mathcal{Z})$. From the above deduction, the l.h.s is $\int_{\mathbb{X}\times\mathcal{Z}} \pi(\mathcal{W}|z)\pi^{\mathscr{G}}(\mathrm{d}x\mathrm{d}z) = \int_{\mathcal{Z}} \pi(\mathcal{X}\times\mathbb{Z}|z)\pi^{\mathbb{Z}}(\mathrm{d}z)$. Defining $\pi(\mathcal{X}|z)$ as $\pi(\mathcal{X}\times\mathbb{Z}|z)$ for any $\mathcal{X} \in \mathscr{X}$, we have:

$$\pi(\mathcal{X}\times\mathcal{Z}) = \int_{\mathcal{Z}} \pi(\mathcal{X}|z)\pi^{\mathbb{Z}}(\mathrm{d}z) = \int_{\mathcal{X}} \pi(\mathcal{Z}|x)\pi^{\mathbb{X}}(\mathrm{d}x),\ \forall \mathcal{X}\times\mathcal{Z} \in \mathscr{X}\times\mathscr{Z}. \tag{11}$$

This is the conditional distribution in the usual sense. Note again that as defined as R-N derivatives, the conditional distributions $\pi(\mathcal{X}|z)$ and $\pi(\mathcal{Z}|x)$ are only $\pi^{\mathbb{Z}}$-unique and $\pi^{\mathbb{X}}$-unique, respectively.

For any $\mathcal{W} \in \mathscr{X}\otimes\mathscr{Z}$, define $\tilde{\pi}(\mathcal{W}) := \int_{\mathbb{Z}} \pi(\mathcal{W}_z|z)\pi^{\mathbb{Z}}(\mathrm{d}z)$. It is easy to verify that $\tilde{\pi}$ is a distribution (probability measure; thus finite and sigma-finite) on $(\mathbb{X}\times\mathbb{Z}, \mathscr{X}\otimes\mathscr{Z})$ [9, p.227], since $\pi(\mathcal{X}|z)$ is a distribution (and thus nonnegative) on $(\mathbb{X}, \mathscr{X})$ for $\pi^{\mathbb{Z}}$-a.e. z [9, Thm. 33.2]. For any $\mathcal{W} = \mathcal{X}\times\mathcal{Z} \in \mathscr{X}\times\mathscr{Z}$, $\tilde{\pi}(\mathcal{W}) = \int_{\mathbb{Z}} \pi(\mathcal{X}|z)\pi^{\mathbb{Z}}(\mathrm{d}z) = \int_{\mathcal{Z}} \pi(\mathcal{X}|z)\pi^{\mathbb{Z}}(\mathrm{d}z) = \pi(\mathcal{X}\times\mathcal{Z})$ due to Eq. (11). So $\tilde{\pi}$ and π agree on the pi-system $\mathscr{X}\times\mathscr{Z}$, which indicates that they agree on $\sigma(\mathscr{X}\times\mathscr{Z}) = \mathscr{X}\otimes\mathscr{Z}$ due to Billingsley [9, Thm. 10.3, Thm. 3.3]. This means that (see the argument in **(ii) (2)** in Supplement A.3 for the second line of the equation):

$$\begin{aligned}\pi(\mathcal{W}) = &\int_{\mathbb{Z}} \pi(\mathcal{W}_z|z)\pi^{\mathbb{Z}}(\mathrm{d}z) = \int_{\mathbb{X}} \pi(\mathcal{W}_x|x)\pi^{\mathbb{X}}(\mathrm{d}x) \\ = &\int_{\mathcal{W}^{\mathbb{Z}}} \pi(\mathcal{W}_z|z)\pi^{\mathbb{Z}}(\mathrm{d}z) = \int_{\mathcal{W}^{\mathbb{X}}} \pi(\mathcal{W}_x|x)\pi^{\mathbb{X}}(\mathrm{d}x),\ \forall \mathcal{W} \in \mathscr{X}\otimes\mathscr{Z}.\end{aligned} \tag{12}$$

Finally, we formalize some definitions in the main text below.

Definition A.1. Consider a general measure space $(\Omega, \mathscr{F}, \mu)$. **(i)** We say that two measurable sets $\mathcal{S}, \tilde{\mathcal{S}} \in \mathscr{F}$ are *μ-a.s. the same*, denoted as "$\mathcal{S} \overset{\mu}{=} \tilde{\mathcal{S}}$", if $\mu(\mathcal{S} \triangle \tilde{\mathcal{S}}) = 0$, where "$\triangle$" denotes the symmetric difference between two sets. **(ii)** We say that $\mathcal{S}$ is a *μ-a.s. subset* of $\mathcal{W}$, denoted as "$\mathcal{S} \subseteq^{\mu} \mathcal{W}$", if $\mu(\mathcal{S} \setminus \mathcal{W}) = 0$.

B Lemmas

B.1 Lemmas for General Probability

Lemma B.1. *Let $\mathcal{O}$ be a measure-zero set, $\mu(\mathcal{O}) = 0$, on a measure space $(\Omega, \mathscr{F}, \mu)$. Then for any measurable set $\mathcal{W}$, we have $\mu(\mathcal{O} \setminus \mathcal{W}) = \mu(\mathcal{W} \cap \mathcal{O}) = 0$, and $\mu(\mathcal{W} \cup \mathcal{O}) = \mu(\mathcal{W} \setminus \mathcal{O}) = \mu(\mathcal{W})$.*

Proof. Due to the monotonicity of a measure [9, Thm. 16.1], we have $\mu(\mathcal{O} \setminus \mathcal{W}) \leqslant \mu(\mathcal{O}) = 0$ and $\mu(\mathcal{W} \cap \mathcal{O}) \leqslant \mu(\mathcal{O}) = 0$, so we get $\mu(\mathcal{O} \setminus \mathcal{W}) = \mu(\mathcal{W} \cap \mathcal{O}) = 0$. Since $\mu(\mathcal{W} \cup \mathcal{O}) = \mu(\mathcal{W} \cup (\mathcal{O} \setminus \mathcal{W}))$ and the two sets are disjoint, it equals to $\mu(\mathcal{W}) + \mu(\mathcal{O} \setminus \mathcal{W})$, which is $\mu(\mathcal{W})$ by the above conclusion. So we get $\mu(\mathcal{W} \cup \mathcal{O}) = \mu(\mathcal{W})$. When applying this conclusion to $\mathcal{W} \setminus \mathcal{O}$, we have $\mu((\mathcal{W} \setminus \mathcal{O}) \cup \mathcal{O}) = \mu(\mathcal{W} \setminus \mathcal{O})$, while the l.h.s is $\mu(\mathcal{W} \cup \mathcal{O})$ which is $\mu(\mathcal{W})$ by the same conclusion. So we get $\mu(\mathcal{W} \setminus \mathcal{O}) = \mu(\mathcal{W})$. $\square$

Lemma B.2. *Let π be an absolutely continuous distribution (probability measure) on a measure space $(\Omega, \mathscr{F}, \mu)$ with a density function f, and let $\mathcal{S} \in \mathscr{F}$ be a measurable set. Then $\pi(\mathcal{S}) = 1$ if and only if $\pi(\mathcal{W}) = \int_{\mathcal{W} \cap \mathcal{S}} f \, \mathrm{d}\mu, \forall \mathcal{W} \in \mathscr{F}$.*

Proof. **"Only if":** Since $\mathcal{S} \subseteq \Omega$, we have $\pi(\Omega \setminus \mathcal{S}) = \pi(\Omega) - \pi(\mathcal{S}) = 0$. For any $\mathcal{W} \in \mathscr{F}$, we have $\pi(\mathcal{W}) = \pi(\mathcal{W} \cap \mathcal{S}) + \pi(\mathcal{W} \cap (\Omega \setminus \mathcal{S}))$, while $0 \leqslant \pi(\mathcal{W} \cap (\Omega \setminus \mathcal{S})) \leqslant \pi(\Omega \setminus \mathcal{S}) = 0$. So we have $\pi(\mathcal{W}) = \pi(\mathcal{W} \cap \mathcal{S}) = \int_{\mathcal{W} \cap \mathcal{S}} f \, \mathrm{d}\mu$.

"If": $1 = \pi(\Omega) = \int_{\Omega \cap \mathcal{S}} f \, \mathrm{d}\mu = \int_{\mathcal{S}} f \, \mathrm{d}\mu = \int_{\mathcal{S} \cap \mathcal{S}} f \, \mathrm{d}\mu = \pi(\mathcal{S})$. □

Lemma B.3. *Let $\mathcal{S}$ and $\tilde{\mathcal{S}}$ be two measurable sets on a measure space $(\Omega, \mathscr{F}, \mu)$ such that $\mathcal{S} \overset{\mu}{=} \tilde{\mathcal{S}}$. Then $\mu(\mathcal{S} \setminus \tilde{\mathcal{S}}) = \mu(\tilde{\mathcal{S}} \setminus \mathcal{S}) = 0$, and $\mu(\mathcal{S}) = \mu(\tilde{\mathcal{S}}) = \mu(\mathcal{S} \cup \tilde{\mathcal{S}}) = \mu(\mathcal{S} \cap \tilde{\mathcal{S}})$.*

Proof. Let $\mathcal{D}^+ := \tilde{\mathcal{S}} \setminus \mathcal{S}$ and $\mathcal{D}^- := \mathcal{S} \setminus \tilde{\mathcal{S}}$. By construction, we have $\mathcal{D}^+ \cap \mathcal{S} = \emptyset$ and $\mathcal{D}^- \subseteq \mathcal{S}$, so we also have $\mathcal{D}^+ \cap \mathcal{D}^- = \emptyset$, and $\tilde{\mathcal{S}} = (\mathcal{S} \setminus \mathcal{D}^-) \cup \mathcal{D}^+ = (\mathcal{S} \cup \mathcal{D}^+) \setminus \mathcal{D}^-$. By definition, $\mathcal{S} \overset{\mu}{=} \tilde{\mathcal{S}}$ indicates $0 = \mu(\mathcal{S} \triangle \tilde{\mathcal{S}}) = \mu(\mathcal{D}^+ \cup \mathcal{D}^-) = \mu(\mathcal{D}^+) + \mu(\mathcal{D}^-)$, so we have both $\mu(\mathcal{D}^+) = 0$ and $\mu(\mathcal{D}^-) = 0$. Subsequently, $\mu(\tilde{\mathcal{S}}) = \mu\big((\mathcal{S} \setminus \mathcal{D}^-) \cup \mathcal{D}^+\big) = \mu(\mathcal{S} \setminus \mathcal{D}^-) + \mu(\mathcal{D}^+) = \mu(\mathcal{S} \setminus \mathcal{D}^-) = \mu(\mathcal{S}) - \mu(\mathcal{D}^- \cap \mathcal{S}) = \mu(\mathcal{S}) - \mu(\mathcal{D}^-) = \mu(\mathcal{S})$, and $\mu(\mathcal{S} \cup \tilde{\mathcal{S}}) = \mu(\mathcal{S} \cup \mathcal{D}^+) = \mu(\mathcal{S}) + \mu(\mathcal{D}^+) = \mu(\mathcal{S})$. Noting also that $\mathcal{S} \cup \tilde{\mathcal{S}} = (\mathcal{S} \cap \tilde{\mathcal{S}}) \cup (\mathcal{S} \triangle \tilde{\mathcal{S}})$ and that this is a disjoint union, we have $\mu(\mathcal{S} \cup \tilde{\mathcal{S}}) = \mu(\mathcal{S} \cap \tilde{\mathcal{S}}) + \mu(\mathcal{S} \triangle \tilde{\mathcal{S}}) = \mu(\mathcal{S} \cap \tilde{\mathcal{S}})$. □

Lemma B.4. *On a measure space $(\Omega, \mathscr{F}, \mu)$, "$\cdot \overset{\mu}{=} \cdot$" is an equivalence relation.*

Proof. Symmetry and reflexivity are obvious. For transitivity, let $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{C}$ be three measurable sets such that $\mathcal{A} \overset{\mu}{=} \mathcal{B}$ and $\mathcal{B} \overset{\mu}{=} \mathcal{C}$. Since $\mathcal{A} \setminus \mathcal{C} = \big((\mathcal{A} \setminus \mathcal{C}) \cap \mathcal{B}\big) \cup \big((\mathcal{A} \setminus \mathcal{C}) \setminus \mathcal{B}\big) = \big(\mathcal{A} \cap (\mathcal{B} \setminus \mathcal{C})\big) \cup \big((\mathcal{A} \setminus \mathcal{B}) \setminus \mathcal{C}\big) \subseteq (\mathcal{B} \setminus \mathcal{C}) \cup (\mathcal{A} \setminus \mathcal{B})$, we have $\mu(\mathcal{A} \setminus \mathcal{C}) \leqslant \mu(\mathcal{B} \setminus \mathcal{C}) + \mu(\mathcal{A} \setminus \mathcal{B}) = 0$ due to Lemma B.3. Similarly, $\mu(\mathcal{C} \setminus \mathcal{A}) = 0$. So $\mu(\mathcal{A} \triangle \mathcal{C}) = \mu(\mathcal{A} \setminus \mathcal{C}) + \mu(\mathcal{C} \setminus \mathcal{A}) = 0$. □

Lemma B.5. *Let $\mathcal{S}$ and $\tilde{\mathcal{S}}$ be two measurable sets on a measure space $(\Omega, \mathscr{F}, \mu)$ such that $\mathcal{S} \overset{\mu}{=} \tilde{\mathcal{S}}$. Then for any measurable set $\mathcal{W}$, we have $\mathcal{S} \cup \mathcal{W} \overset{\mu}{=} \tilde{\mathcal{S}} \cup \mathcal{W}$, $\mathcal{S} \cap \mathcal{W} \overset{\mu}{=} \tilde{\mathcal{S}} \cap \mathcal{W}$, $\mathcal{S} \setminus \mathcal{W} \overset{\mu}{=} \tilde{\mathcal{S}} \setminus \mathcal{W}$ and $\mathcal{W} \setminus \mathcal{S} \overset{\mu}{=} \mathcal{W} \setminus \tilde{\mathcal{S}}$.*

Proof. Let $\mathcal{D}^+ := \tilde{\mathcal{S}} \setminus \mathcal{S}$ and $\mathcal{D}^- := \mathcal{S} \setminus \tilde{\mathcal{S}}$. By Lemma B.3, we have $\mu(\mathcal{D}^+) = 0$ and $\mu(\mathcal{D}^-) = 0$.

For any measurable set $\mathcal{W}$, we have $(\tilde{\mathcal{S}} \cup \mathcal{W}) \setminus (\mathcal{S} \cup \mathcal{W}) = \tilde{\mathcal{S}} \setminus \mathcal{S} \setminus \mathcal{W} = \mathcal{D}^+ \setminus \mathcal{W}$, and similarly $(\mathcal{S} \cup \mathcal{W}) \setminus (\tilde{\mathcal{S}} \cup \mathcal{W}) = \mathcal{D}^- \setminus \mathcal{W}$. So $\mu\big((\mathcal{S} \cup \mathcal{W}) \triangle (\tilde{\mathcal{S}} \cup \mathcal{W})\big) = \mu\big(\big((\mathcal{S} \cup \mathcal{W}) \setminus (\tilde{\mathcal{S}} \cup \mathcal{W})\big) \cup \big((\tilde{\mathcal{S}} \cup \mathcal{W}) \setminus (\mathcal{S} \cup \mathcal{W})\big)\big) = \mu\big((\mathcal{D}^- \setminus \mathcal{W}) \cup (\mathcal{D}^+ \setminus \mathcal{W})\big) = \mu(\mathcal{D}^- \setminus \mathcal{W}) + \mu(\mathcal{D}^+ \setminus \mathcal{W}) \leqslant \mu(\mathcal{D}^-) + \mu(\mathcal{D}^+) = 0$, that is $\mathcal{S} \cup \mathcal{W} \overset{\mu}{=} \tilde{\mathcal{S}} \cup \mathcal{W}$.

Since $(\tilde{\mathcal{S}} \cap \mathcal{W}) \setminus (\mathcal{S} \cap \mathcal{W}) = (\tilde{\mathcal{S}} \setminus \mathcal{S}) \cap \mathcal{W} = \mathcal{D}^+ \cap \mathcal{W}$ and similarly $(\mathcal{S} \cap \mathcal{W}) \setminus (\tilde{\mathcal{S}} \cap \mathcal{W}) = \mathcal{D}^- \cap \mathcal{W}$, we have $\mu\big((\mathcal{S} \cap \mathcal{W}) \triangle (\tilde{\mathcal{S}} \cap \mathcal{W})\big) = \mu\big(\big((\mathcal{S} \cap \mathcal{W}) \setminus (\tilde{\mathcal{S}} \cap \mathcal{W})\big) \cup \big((\tilde{\mathcal{S}} \cap \mathcal{W}) \setminus (\mathcal{S} \cap \mathcal{W})\big)\big) = \mu\big((\mathcal{D}^- \cap \mathcal{W}) \cup (\mathcal{D}^+ \cap \mathcal{W})\big) = \mu(\mathcal{D}^- \cap \mathcal{W}) + \mu(\mathcal{D}^+ \cap \mathcal{W}) \leqslant \mu(\mathcal{D}^-) + \mu(\mathcal{D}^+) = 0$, so $\mathcal{S} \cap \mathcal{W} \overset{\mu}{=} \tilde{\mathcal{S}} \cap \mathcal{W}$.

Since $(\tilde{\mathcal{S}} \setminus \mathcal{W}) \setminus (\mathcal{S} \setminus \mathcal{W}) = \tilde{\mathcal{S}} \setminus \mathcal{W} \setminus \mathcal{S} = \tilde{\mathcal{S}} \setminus \mathcal{S} \setminus \mathcal{W} = \mathcal{D}^+ \setminus \mathcal{W}$ and similarly $(\mathcal{S} \setminus \mathcal{W}) \setminus (\tilde{\mathcal{S}} \setminus \mathcal{W}) = \mathcal{D}^- \setminus \mathcal{W}$, we have $\mu\big((\mathcal{S} \setminus \mathcal{W}) \triangle (\tilde{\mathcal{S}} \setminus \mathcal{W})\big) = \mu\big(\big((\mathcal{S} \setminus \mathcal{W}) \setminus (\tilde{\mathcal{S}} \setminus \mathcal{W})\big) \cup \big((\tilde{\mathcal{S}} \setminus \mathcal{W}) \setminus (\mathcal{S} \setminus \mathcal{W})\big)\big) = \mu\big((\mathcal{D}^- \setminus \mathcal{W}) \cup (\mathcal{D}^+ \setminus \mathcal{W})\big) = \mu(\mathcal{D}^- \setminus \mathcal{W}) + \mu(\mathcal{D}^+ \setminus \mathcal{W}) \leqslant \mu(\mathcal{D}^-) + \mu(\mathcal{D}^+) = 0$, so $\mathcal{S} \setminus \mathcal{W} \overset{\mu}{=} \tilde{\mathcal{S}} \setminus \mathcal{W}$.

Since $(\mathcal{W} \setminus \tilde{\mathcal{S}}) \setminus (\mathcal{W} \setminus \mathcal{S}) = \mathcal{W} \setminus (\mathcal{W} \setminus \mathcal{S}) \setminus \tilde{\mathcal{S}} = (\mathcal{W} \cap \mathcal{S}) \setminus \tilde{\mathcal{S}} = (\mathcal{S} \setminus \tilde{\mathcal{S}}) \cap \mathcal{W} = \mathcal{D}^- \cap \mathcal{W}$ and similarly $(\mathcal{W} \setminus \mathcal{S}) \setminus (\mathcal{W} \setminus \tilde{\mathcal{S}}) = \mathcal{D}^+ \cap \mathcal{W}$, we have $\mu\big((\mathcal{W} \setminus \mathcal{S}) \triangle (\mathcal{W} \setminus \tilde{\mathcal{S}})\big) = \mu\big(\big((\mathcal{W} \setminus \mathcal{S}) \setminus (\mathcal{W} \setminus \tilde{\mathcal{S}})\big) \cup \big((\mathcal{W} \setminus \tilde{\mathcal{S}}) \setminus (\mathcal{W} \setminus \mathcal{S})\big)\big) = \mu\big((\mathcal{D}^+ \cap \mathcal{W}) \cup (\mathcal{D}^- \cap \mathcal{W})\big) = \mu(\mathcal{D}^+ \cap \mathcal{W}) + \mu(\mathcal{D}^- \cap \mathcal{W}) \leqslant \mu(\mathcal{D}^+) + \mu(\mathcal{D}^-) = 0$, so $\mathcal{W} \setminus \mathcal{S} \overset{\mu}{=} \mathcal{W} \setminus \tilde{\mathcal{S}}$. □

Definition B.6. We say that a set satisfying a certain condition is *μ-unique*, if for any two such sets $\mathcal{S}$ and $\tilde{\mathcal{S}}$, it holds that $\mathcal{S} \overset{\mu}{=} \tilde{\mathcal{S}}$.

Lemma B.7. *Let π be an absolutely continuous distribution (probability measure) on a measure space $(\Omega, \mathscr{F}, \mu)$ with a density function f. If a set $\mathcal{S} \in \mathscr{F}$ satisfies $\pi(\mathcal{S}) = 1$ and that $f > 0$, μ-a.e. on $\mathcal{S}$, then such an $\mathcal{S}$ is μ-unique.*

***Proof*.** Suppose we have two such sets $\mathcal{S}$ and $\tilde{\mathcal{S}}$. By Lemma B.2, we know that for any $\mathcal{W} \in \mathscr{F}$, $\pi(\mathcal{W}) = \int_{\mathcal{W}\cap\mathcal{S}} f \,\mathrm{d}\mu = \int_{\mathcal{W}} \mathbb{I}_{\mathcal{S}} f \,\mathrm{d}\mu = \int_{\mathcal{W}} \mathbb{I}_{\tilde{\mathcal{S}}} f \,\mathrm{d}\mu$. So by Billingsley [9, Thm. 16.10(ii)], we know that $\mathbb{I}_{\mathcal{S}} f = \mathbb{I}_{\tilde{\mathcal{S}}} f$, μ-a.e.

Since $f > 0$, μ-a.e. on $\mathcal{S}$, we know that $\mathbb{I}_{\mathcal{S}} = \mathbb{I}_{\tilde{\mathcal{S}}}$, μ-a.e. on $\mathcal{S}$. This means that $\mu\{\omega \in \mathcal{S} \mid \mathbb{I}_{\mathcal{S}} \neq \mathbb{I}_{\tilde{\mathcal{S}}}\} = \mu\{\omega \in \mathcal{S} \mid \omega \notin \tilde{\mathcal{S}}\} = \mu(\mathcal{S} \setminus \tilde{\mathcal{S}}) = 0$. Symmetrically, since $f > 0$, μ-a.e. also on $\tilde{\mathcal{S}}$, we know that $\mu(\tilde{\mathcal{S}} \setminus \mathcal{S}) = 0$. So we have $\mu(\mathcal{S}\triangle\tilde{\mathcal{S}}) = \mu((\mathcal{S}\setminus\tilde{\mathcal{S}})\cup(\tilde{\mathcal{S}}\setminus\mathcal{S})) = \mu(\mathcal{S}\setminus\tilde{\mathcal{S}}) + \mu(\tilde{\mathcal{S}}\setminus\mathcal{S}) = 0$, which means that $\mathcal{S} \overset{\mu}{=} \tilde{\mathcal{S}}$. □

The μ-unique set $\mathcal{S}$ in the lemma serves as another form of the *support* of a distribution. The standard definition of the support requires a topological structure and $\mathscr{F}$ is the corresponding Borel sigma-field. If given absolute continuity $\pi \ll \mu$, this lemma enables the generality that does not require a topological structure. The condition $\pi(\mathcal{S}) = 1$ prevents $\mathcal{S}$ to be too small, while the condition that $f > 0$, μ-a.e. on $\mathcal{S}$ prevents $\mathcal{S}$ to be too large.

Definition B.8 (support of an absolutely continuous distribution (without topology))**.** Define the *support* of an absolutely continuous distribution (probability measure) π on a measure space $(\Omega, \mathscr{F}, \mu)$, as the μ-unique set $\mathcal{S} \in \mathscr{F}$ such that $\pi(\mathcal{S}) = 1$ and for any density function f of π, it holds that $f > 0$, μ-a.e. on $\mathcal{S}$.

B.2 Lemmas for Product Probability

In this subsection and the following, let $(\mathbb{X}\times\mathbb{Z}, \mathscr{X}\otimes\mathscr{Z}, \xi\otimes\zeta)$ be the product measure space by the two individual ones $(\mathbb{X}, \mathscr{X}, \xi)$ and $(\mathbb{Z}, \mathscr{Z}, \zeta)$, where ξ and ζ are sigma-finite.

Lemma B.9. *For a measure π on the product measure space $(\mathbb{X}\times\mathbb{Z}, \mathscr{X}\otimes\mathscr{Z}, \xi\otimes\zeta)$, if $\pi \ll \xi\otimes\zeta$, then $\pi^{\mathbb{X}} \ll \xi$ and $\pi^{\mathbb{Z}} \ll \zeta$.*

***Proof*.** For any $\mathcal{X} \in \mathscr{X}$ such that $\xi(\mathcal{X}) = 0$, we have $(\xi\otimes\zeta)(\mathcal{X}\times\mathbb{Z}) = \xi(\mathcal{X})\zeta(\mathbb{Z}) = 0$, where the last equality is verified in **(ii) (1)** in Supplement A.3 when $\zeta(\mathbb{Z}) = \infty$. Since $\pi \ll \xi\otimes\zeta$, this means that $\pi(\mathcal{X}\times\mathbb{Z}) = \pi^{\mathbb{X}}(\mathcal{X}) = 0$. So $\pi^{\mathbb{X}} \ll \xi$. Similarly, $\pi^{\mathbb{Z}} \ll \zeta$. □

Lemma B.10. *For an assertion $t(x, z)$ on $\mathcal{W} \in \mathscr{X}\otimes\mathscr{Z}$, $t(x, z)$ holds $\xi\otimes\zeta$-a.e. on $\mathcal{W}$, if and only if $t(x, z)$ holds ξ-a.e. on $\mathcal{W}_z$, for ζ-a.e. z on $\mathcal{W}^{\mathbb{Z}}$.*

***Proof*.** By the definition of "$t(x, z)$ holds $\xi\otimes\zeta$-a.e. on $\mathcal{W}$", we have:

$$(\xi\otimes\zeta)\{(x, z) \in \mathcal{W} \mid \neg t(x, z)\} = 0 \qquad \text{(Since } \xi \text{ and } \zeta \text{ are sigma-finite, from Eq. (7),)}$$

$$\iff \int_{\mathcal{W}^{\mathbb{Z}}} \xi\{x \in \mathcal{W}_z \mid \neg t(x, z)\}\zeta(\mathrm{d}z) = 0$$

(Since $\xi(\cdot)$ is nonnegative, from Billingsley [9, Thm. 15.2],)

$\iff \xi\{x \in \mathcal{W}_z \mid \neg t(x, z)\} = 0$, for ζ-a.e. z on $\mathcal{W}^{\mathbb{Z}}$,

which is "$t(x, z)$ holds ξ-a.e. on $\mathcal{W}_z$, for ζ-a.e. z on $\mathcal{W}^{\mathbb{Z}}$". □

Lemma B.11. *Let $\mathcal{X}, \tilde{\mathcal{X}} \in \mathscr{X}$ such that $\mathcal{X} \overset{\xi}{=} \tilde{\mathcal{X}}$. Then $\mathcal{X}\times\mathbb{Z} \overset{\xi\otimes\zeta}{=} \tilde{\mathcal{X}}\times\mathbb{Z}$.*

***Proof*.** Since $(\mathcal{X}\times\mathbb{Z})\triangle(\tilde{\mathcal{X}}\times\mathbb{Z}) = \big((\mathcal{X}\times\mathbb{Z})\setminus(\tilde{\mathcal{X}}\times\mathbb{Z})\big)\cup\big((\tilde{\mathcal{X}}\times\mathbb{Z})\setminus(\mathcal{X}\times\mathbb{Z})\big) = \big((\mathcal{X}\setminus\tilde{\mathcal{X}})\cup(\tilde{\mathcal{X}}\setminus\mathcal{X})\big)\times\mathbb{Z}$, we can verify that $(\xi\otimes\zeta)\big((\mathcal{X}\times\mathbb{Z})\triangle(\tilde{\mathcal{X}}\times\mathbb{Z})\big) = (\xi\otimes\zeta)\big(\big((\mathcal{X}\setminus\tilde{\mathcal{X}})\cup(\tilde{\mathcal{X}}\setminus\mathcal{X})\big)\times\mathbb{Z}\big) = \xi\big((\mathcal{X}\setminus\tilde{\mathcal{X}})\cup(\tilde{\mathcal{X}}\setminus\mathcal{X})\big)\zeta(\mathbb{Z}) = \xi(\mathcal{X}\triangle\tilde{\mathcal{X}})\zeta(\mathbb{Z}) = 0$, where the last equality is verified in **(ii) (1)** in Supplement A.3 when $\zeta(\mathbb{Z}) = \infty$. □

B.3 Lemmas for $\xi\otimes\zeta$-Complete Component

Echoing Def. 2.2, a set $\mathcal{S} \in \mathscr{X}\otimes\mathscr{Z}$ is called a $\xi\otimes\zeta$*-complete component* of $\mathcal{W} \in \mathscr{X}\otimes\mathscr{Z}$, if

$$\mathcal{S}^{\sharp} \cap \mathcal{W} \overset{\xi\otimes\zeta}{=} \mathcal{S}, \text{where } \mathcal{S}^{\sharp} := \mathcal{S}^{\mathbb{X}}\times\mathbb{Z} \cup \mathbb{X}\times\mathcal{S}^{\mathbb{Z}}. \tag{13}$$

This means that $\mathcal{S}$ is complete under *stretching* and intersecting with $\mathcal{W}$.

Lemma B.12. *Let $\mathcal{S}$ be a $\xi\otimes\zeta$-complete component of $\mathcal{W}$. Then $\mathcal{S} \subseteq^{\xi\otimes\zeta} \mathcal{W}$.*

***Proof*.** By construction, we have $\mathcal{S} \subseteq \mathcal{S}^{\sharp}$ so $\mathcal{S}\setminus\mathcal{W} = \mathcal{S}\setminus(\mathcal{S}\cap\mathcal{W}) = \mathcal{S}\setminus(\mathcal{S}^{\sharp}\cap\mathcal{W})$. Hence, $(\xi\otimes\zeta)(\mathcal{S}\setminus\mathcal{W}) = (\xi\otimes\zeta)\big(\mathcal{S}\setminus(\mathcal{S}^{\sharp}\cap\mathcal{W})\big) = 0$ by definition Eq. (13) and Lemma B.3. □

Example B.13. Note that when $\mathcal{S}$ is a $\xi\otimes\zeta$-complete component of $\mathcal{W}$, it may not hold that $\mathcal{S}^{\mathbb{X}} \subseteq^{\xi} \mathcal{W}^{\mathbb{X}}$ and $\mathcal{S}^{\mathbb{Z}} \subseteq^{\zeta} \mathcal{W}^{\mathbb{Z}}$. Fig. 6 shows an example, where $(\mathbb{X}, \mathscr{X}, \xi)$ and $(\mathbb{Z}, \mathscr{Z}, \zeta)$ are the one dimensional Euclidean spaces with line Borel sigma-field and line Lebesgue measure, $(\mathbb{R}, \mathscr{R}, \lambda)$, and $\mathcal{W} := [0,1]^2$ and $\mathcal{S} := [0,1]^2 \cup ([1,2]\times\{\frac{1}{2}\})$. We have $\mathcal{S}^{\mathbb{X}} = [0,2]$ so $\mathcal{S}^{\sharp} = ([0,2]\times\mathbb{R}) \cup (\mathbb{R}\times[0,1])$ and $\mathcal{S}^{\sharp} \cap \mathcal{W} = \mathcal{W}$. Since $\mathcal{S}\triangle\mathcal{W} = [1,2]\times\{\frac{1}{2}\}$ is a line segment that has measure zero under the plane Lebesgue measure $\xi\otimes\zeta = \lambda^2$, we have $\mathcal{S} \overset{\xi\otimes\zeta}{=} \mathcal{W}$ so $\mathcal{S}$ is a $\xi\otimes\zeta$-complete component of $\mathcal{W}$. But $\xi(\mathcal{S}^{\mathbb{X}} \setminus \mathcal{W}^{\mathbb{X}}) = \lambda([0,2] \setminus [0,1]) = \lambda(1,2] = 1$ is not zero, so $\mathcal{S}^{\mathbb{X}} \subseteq^{\xi} \mathcal{W}^{\mathbb{X}}$ does not hold.

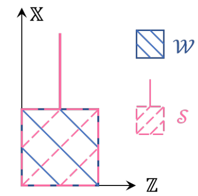


Figure 6: Example B.13 showing that a $\xi\otimes\zeta$-complete component of $\mathcal{W}$ may not have its projection be an a.s. subset of that of $\mathcal{W}$.

Lemma B.14. *Let $\mathcal{S}$ be a $\xi\otimes\zeta$-complete component of $\mathcal{W}$, and $\tilde{\mathcal{S}}$ be a measurable set such that $\tilde{\mathcal{S}} \overset{\xi\otimes\zeta}{=} \mathcal{S}$, $\tilde{\mathcal{S}}^{\mathbb{X}} \overset{\xi}{=} \mathcal{S}^{\mathbb{X}}$ and $\tilde{\mathcal{S}}^{\mathbb{Z}} \overset{\zeta}{=} \mathcal{S}^{\mathbb{Z}}$. Then this $\tilde{\mathcal{S}}$ is also a $\xi\otimes\zeta$-complete component of $\mathcal{W}$.*

Proof. By Lemma B.11, we know that $\tilde{\mathcal{S}}^{\mathbb{X}}\times\mathbb{Z} \overset{\xi\otimes\zeta}{=} \mathcal{S}^{\mathbb{X}}\times\mathbb{Z}$, $\mathbb{X}\times\tilde{\mathcal{S}}^{\mathbb{Z}} \overset{\xi\otimes\zeta}{=} \mathbb{X}\times\mathcal{S}^{\mathbb{Z}}$. Repeatedly applying Lemma B.5, we have $\tilde{\mathcal{S}}^{\sharp} := \tilde{\mathcal{S}}^{\mathbb{X}}\times\mathbb{Z} \cup \mathbb{X}\times\tilde{\mathcal{S}}^{\mathbb{Z}} \overset{\xi\otimes\zeta}{=} \mathcal{S}^{\mathbb{X}}\times\mathbb{Z} \cup \mathbb{X}\times\tilde{\mathcal{S}}^{\mathbb{Z}} \overset{\xi\otimes\zeta}{=} \mathcal{S}^{\mathbb{X}}\times\mathbb{Z} \cup \mathbb{X}\times\mathcal{S}^{\mathbb{Z}} =: \mathcal{S}^{\sharp}$, and $\tilde{\mathcal{S}}^{\sharp} \cap \mathcal{W} \overset{\xi\otimes\zeta}{=} \mathcal{S}^{\sharp} \cap \mathcal{W}$, which $\overset{\xi\otimes\zeta}{=} \mathcal{S} \overset{\xi\otimes\zeta}{=} \tilde{\mathcal{S}}$. From the transitivity (Lemma B.4), we have $\tilde{\mathcal{S}}^{\sharp} \cap \mathcal{W} \overset{\xi\otimes\zeta}{=} \tilde{\mathcal{S}}$. $\square$

Example B.15. Note that only the $\tilde{\mathcal{S}} \overset{\xi\otimes\zeta}{=} \mathcal{S}$ condition is not sufficient. Fig. 7 shows such an example, where $(\mathbb{X}, \mathscr{X}, \xi)$ and $(\mathbb{Z}, \mathscr{Z}, \zeta)$ are the one dimensional Euclidean spaces with line Borel sigma-field and line Lebesgue measure, $(\mathbb{R}, \mathscr{R}, \lambda)$, and $\mathcal{W} := [0,1]^2 \cup [1,2]^2$, $\mathcal{S} := [0,1]^2$, and $\tilde{\mathcal{S}} := [0,1]^2 \cup ([1,2]\times\{\frac{1}{2}\})$. We have $\mathcal{S}^{\sharp} = ([0,1]\times\mathbb{R}) \cup (\mathbb{R}\times[0,1])$ so $\mathcal{S}^{\sharp} \cap \mathcal{W} = \mathcal{S}$, justifying that $\mathcal{S}$ is a $\xi\otimes\zeta$-complete component of $\mathcal{W}$. On the other hand, since $\mathcal{S}\triangle\tilde{\mathcal{S}} = [1,2]\times\{\frac{1}{2}\}$ is a line segment that has measure zero under the plane Lebesgue measure $\xi\otimes\zeta = \lambda^2$, we have $\tilde{\mathcal{S}} \overset{\xi\otimes\zeta}{=} \mathcal{S}$. But $\tilde{\mathcal{S}}^{\mathbb{X}} = [0,2]$ so $\tilde{\mathcal{S}}^{\sharp} = ([0,2]\times\mathbb{R}) \cup (\mathbb{R}\times[0,1])$, which leads to $\tilde{\mathcal{S}}^{\sharp} \cap \mathcal{W} = \mathcal{W}$. Since $\tilde{\mathcal{S}}\triangle\mathcal{W} = ([1,2]\times\{\frac{1}{2}\}) \cup ([1,2]\times[1,2])$ has a nonzero measure under λ^2 (it equals to 1), we know that $\tilde{\mathcal{S}}$ is not a $\xi\otimes\zeta$-complete component of $\mathcal{W}$.

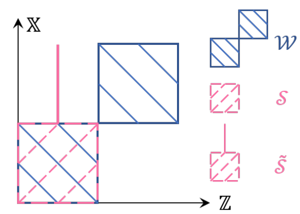


Figure 7: Example B.15 showing that in Lem. B.14, only being $\xi\otimes\zeta$-a.s. the same as a $\xi\otimes\zeta$-complete component $\tilde{\mathcal{S}}$ of $\mathcal{W}$ is not sufficient for $\tilde{\mathcal{S}}$ to be also a $\xi\otimes\zeta$-complete component of $\mathcal{W}$.

Lemma B.16. *Let $\mathcal{S}$ be a $\xi\otimes\zeta$-complete component of $\mathcal{W}$, and f be an either nonnegative or $\xi\otimes\zeta$-integrable function on $\mathbb{X}\times\mathbb{Z}$. Then for any measurable sets $\mathcal{Z} \subseteq \mathcal{S}^{\mathbb{Z}}$ and $\mathcal{X} \subseteq \mathcal{S}^{\mathbb{X}}$, we have:*

$$\int_{\mathcal{Z}} \int_{\mathcal{W}_z} f(x,z)\xi(\mathrm{d}x)\zeta(\mathrm{d}z) = \int_{\mathcal{Z}} \int_{\mathcal{S}_z} f(x,z)\xi(\mathrm{d}x)\zeta(\mathrm{d}z),$$

$$\int_{\mathcal{X}} \int_{\mathcal{W}_x} f(x,z)\zeta(\mathrm{d}z)\xi(\mathrm{d}x) = \int_{\mathcal{X}} \int_{\mathcal{S}_x} f(x,z)\zeta(\mathrm{d}z)\xi(\mathrm{d}x).$$

Particularly, $\int_{\mathcal{S}^{\mathbb{Z}}} \int_{\mathcal{W}_z} f(x,z)\xi(\mathrm{d}x)\zeta(\mathrm{d}z) = \int_{\mathcal{S}^{\mathbb{X}}} \int_{\mathcal{W}_x} f(x,z)\zeta(\mathrm{d}z)\xi(\mathrm{d}x) = \int_{\mathcal{S}} f(x,z)(\xi\otimes\zeta)(\mathrm{d}x\mathrm{d}z)$.

Proof. Since $\mathcal{S}$ is a $\xi\otimes\zeta$-complete component of $\mathcal{W}$, Eq. (13) holds. By Lemma B.10, we know that for ζ-a.e. z on $\mathbb{Z}$, $\xi\big((\mathcal{S}^{\sharp} \cap \mathcal{W})\triangle\mathcal{S}\big)_z = \xi\big((\mathcal{S}^{\sharp}_z \cap \mathcal{W}_z)\triangle\mathcal{S}_z\big) = 0$. Noting that $\mathcal{S}^{\sharp}_z = \mathbb{X}$ for any $z \in \mathcal{S}^{\mathbb{Z}}$, this subsequently means that $\xi(\mathcal{W}_z\triangle\mathcal{S}_z) = 0$ for ζ-a.e. z on $\mathcal{S}^{\mathbb{Z}}$. By the additivity of integrals over a countable partition [9, Thm. 16.9] and that the integral over a measure-zero set is zero [9, p.226], we have $\int_{\mathcal{W}_z} f(x,z)\xi(\mathrm{d}x) = \int_{\mathcal{S}_z} f(x,z)\xi(\mathrm{d}x)$ for ζ-a.e. z on $\mathcal{S}^{\mathbb{Z}}$. Since a.e.-equal functions have the same integral [9, Thm. 15.2(v)], we have for any measurable $\mathcal{Z} \subseteq \mathcal{S}^{\mathbb{Z}}$, $\int_{\mathcal{Z}} \int_{\mathcal{W}_z} f(x,z)\xi(\mathrm{d}x)\zeta(\mathrm{d}z) = \int_{\mathcal{Z}} \int_{\mathcal{S}_z} f(x,z)\xi(\mathrm{d}x)\zeta(\mathrm{d}z)$. Similarly, for any measurable $\mathcal{X} \subseteq \mathcal{S}^{\mathbb{X}}$, $\int_{\mathcal{X}} \int_{\mathcal{W}_x} f(x,z)\zeta(\mathrm{d}z)\xi(\mathrm{d}x) = \int_{\mathcal{X}} \int_{\mathcal{S}_x} f(x,z)\zeta(\mathrm{d}z)\xi(\mathrm{d}x)$.

For $\mathcal{Z} = \mathcal{S}^{\mathbb{Z}}$, we have $\int_{\mathcal{S}^{\mathbb{Z}}} \int_{\mathcal{W}_z} f(x,z)\xi(\mathrm{d}x)\zeta(\mathrm{d}z) = \int_{\mathcal{S}^{\mathbb{Z}}} \int_{\mathcal{S}_z} f(x,z)\xi(\mathrm{d}x)\zeta(\mathrm{d}z)$, which is $\int_{\mathcal{S}} f(x,z)(\xi\otimes\zeta)(\mathrm{d}x\mathrm{d}z)$ by the generalized form Eq. (9) of Fubini's theorem. Similarly, $\int_{\mathcal{S}^{\mathbb{X}}} \int_{\mathcal{W}_x} f(x,z)\zeta(\mathrm{d}z)\xi(\mathrm{d}x) = \int_{\mathcal{S}} f(x,z)(\xi\otimes\zeta)(\mathrm{d}x\mathrm{d}z)$. $\square$

C Proofs

Recall that $(\mathbb{X}\times\mathbb{Z}, \mathscr{X}\otimes\mathscr{Z}, \xi\otimes\zeta)$ is the product measure space by the two individual ones $(\mathbb{X}, \mathscr{X}, \xi)$ and $(\mathbb{Z}, \mathscr{Z}, \zeta)$, where ξ and ζ are sigma-finite.

C.1 The Joint-Conditional Absolute Continuity Lemma

Although this lemma is not formally presented in the main text, we highlight it here since it answers an important question and the answer is not straightforward.

The lemma reveals the relation between the absolute continuity of a joint π and that of its conditionals $\pi(\cdot|z)$, $\pi(\cdot|x)$. Roughly, the former guarantees the latter on the supports of the marginals, and the reverse also holds, allowing one to safely use the density-function calculus for deduction. But given two conditionals, one does not have the knowledge on the marginals *a priori*. For a more useful sufficient condition, one may consider the absolute continuity of the conditionals for ζ-a.e. z and ξ-a.e. x. Unfortunately this is not sufficient, and an example (C.2) is given after the proof. The lemma shows it is sufficient if the absolute continuity of one of the conditionals, say $\pi(\cdot|z)$, holds for *any* $z \in \mathbb{Z}$. The condition in the compatibility criterion Thm. 2.3 is also inspired from this lemma.

Lemma C.1 (joint-conditional absolute continuity)**.** ***(i)*** *For a joint distribution π on $(\mathbb{X}\times\mathbb{Z}, \mathscr{X}\otimes\mathscr{Z})$, it is absolutely continuous $\pi \ll \xi\otimes\zeta$ if and only if $\pi(\cdot|z) \ll \xi$ for $\pi^{\mathbb{Z}}$-a.e. z and $\pi(\cdot|x) \ll \zeta$ for $\pi^{\mathbb{X}}$-a.e. x.* ***(ii)*** *As a sufficient condition, $\pi \ll \xi\otimes\zeta$ if $\pi(\cdot|z) \ll \xi$ for ζ-a.e. z and $\pi(\cdot|x) \ll \zeta$ for* any *$x \in \mathbb{X}$ (or for* any *$z \in \mathbb{Z}$ and ξ-a.e. x).*

For conclusion (i):

Proof. **"Only if":** Consider any $\mathcal{X} \in \mathscr{X}$ such that $\xi(\mathcal{X}) = 0$. From the definition of conditional distribution Eq. (11), we have $\pi^{\mathbb{X}}(\mathcal{X}) = \pi(\mathcal{X}\times\mathbb{Z}) = \int_{\mathbb{Z}} \pi(\mathcal{X}|z)\pi^{\mathbb{Z}}(\mathrm{d}z) = 0$, so $\pi(\mathcal{X}|z) = 0$ for $\pi^{\mathbb{Z}}$-a.e. z since $\pi(\mathcal{X}|z)$ is nonnegative [9, Thm. 15.2(ii)]. This means that $\pi(\cdot|z) \ll \xi$ for $\pi^{\mathbb{Z}}$-a.e. z. The same arguments apply symmetrically to $\pi(\cdot|x)$.

Note that since $\pi(\cdot|z)$ is defined as the R-N derivative, it is allowed to take any nonnegative value on a $\pi^{\mathbb{Z}}$-measure-zero set. So we cannot guarantee its behavior for *any* $z \in \mathbb{Z}$.

"If": Consider any $\mathcal{Z} \in \mathscr{Z}$ such that $\zeta(\mathcal{Z}) = 0$. Since $\pi(\cdot|x) \ll \zeta$ for $\pi^{\mathbb{X}}$-a.e. x, we have $\pi(\mathcal{Z}|x) = 0$ for $\pi^{\mathbb{X}}$-a.e. x. So from Eq. (11) we have $\pi^{\mathbb{Z}}(\mathcal{Z}) = \pi(\mathbb{X}\times\mathcal{Z}) = \int_{\mathbb{X}} \pi(\mathcal{Z}|x)\pi^{\mathbb{X}}(\mathrm{d}x) = 0$ [9, Thm. 15.2(i)]. This indicates that $\pi^{\mathbb{Z}} \ll \zeta$.

Now consider any $\mathcal{W} \in \mathscr{X}\otimes\mathscr{Z}$ such that $(\xi\otimes\zeta)(\mathcal{W}) = 0$. By the definition of product measure Eq. (6) [9, Thm. 18.2], we have $(\xi\otimes\zeta)(\mathcal{W}) = \int_{\mathbb{Z}} \xi(\mathcal{W}_z)\zeta(\mathrm{d}z) = 0$, so $\xi(\mathcal{W}_z) = 0$ for ζ-a.e. z since $\xi(\mathcal{W}_z)$ is nonnegative [9, Thm. 15.2(ii)]. Due to that $\pi^{\mathbb{Z}} \ll \zeta$, this means that $\xi(\mathcal{W}_z) = 0$ for $\pi^{\mathbb{Z}}$-a.e. z. Since $\pi(\cdot|z) \ll \xi$ for $\pi^{\mathbb{Z}}$-a.e. z, this in turn means that $\pi(\mathcal{W}_z|z) = 0$ for $\pi^{\mathbb{Z}}$-a.e. z. Subsequently, we have $\int_{\mathbb{Z}} \pi(\mathcal{W}_z|z)\pi^{\mathbb{Z}}(\mathrm{d}z) = 0$ [9, Thm. 15.2(i)], which is $\pi(\mathcal{W}) = 0$ by Eq. (12). So we get $\pi \ll \xi\otimes\zeta$. □

For conclusion (ii):

Proof. Consider any $\mathcal{Z} \in \mathscr{Z}$ such that $\zeta(\mathcal{Z}) = 0$. Since $\pi(\cdot|x) \ll \zeta$ for any $x \in \mathbb{X}$, we know that $\pi(\mathcal{Z}|x) = 0$ for any $x \in \mathbb{X}$. So from Eq. (11) we have $\pi^{\mathbb{Z}}(\mathcal{Z}) = \pi(\mathbb{X}\times\mathcal{Z}) = \int_{\mathbb{X}} \pi(\mathcal{Z}|x)\pi^{\mathbb{X}}(\mathrm{d}x) = 0$. This indicates that $\pi^{\mathbb{Z}} \ll \zeta$.

Now consider any $\mathcal{W} \in \mathscr{X}\otimes\mathscr{Z}$ such that $(\xi\otimes\zeta)(\mathcal{W}) = 0$. By the definition of product measure Eq. (6) [9, Thm. 18.2], we have $(\xi\otimes\zeta)(\mathcal{W}) = \int_{\mathbb{Z}} \xi(\mathcal{W}_z)\zeta(\mathrm{d}z) = 0$, so $\xi(\mathcal{W}_z) = 0$ for ζ-a.e. z since $\xi(\mathcal{W}_z)$ is nonnegative [9, Thm. 15.2(ii)]. Due to that $\pi(\cdot|z) \ll \xi$ for ζ-a.e. z, this means that $\pi(\mathcal{W}_z|z) = 0$ for ζ-a.e. z. Since $\pi^{\mathbb{Z}} \ll \zeta$, this in turn means that $\pi(\mathcal{W}_z|z) = 0$ for $\pi^{\mathbb{Z}}$-a.e. z. Subsequently, we have $\int_{\mathbb{Z}} \pi(\mathcal{W}_z|z)\pi^{\mathbb{Z}}(\mathrm{d}z) = 0$ [9, Thm. 15.2(i)], which is $\pi(\mathcal{W}) = 0$ by Eq. (12). So we get $\pi \ll \xi\otimes\zeta$. The same arguments apply symmetrically when $\pi(\cdot|z) \ll \xi$ for *any* $z \in \mathbb{Z}$ and $\pi(\cdot|x) \ll \zeta$ for ξ-a.e. x. □

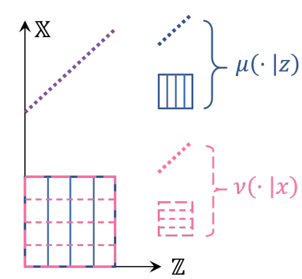


Figure 8: Illustration of the conditionals in Eq. (14) in Example C.2. Both conditionals are absolutely continuous for ζ-a.e. z or ξ-a.e. x, but they allow a compatible joint that is not absolutely continuous w.r.t $\xi\otimes\zeta$.

Example C.2. To see why it is not sufficient if the two conditionals are absolutely continuous only for ζ-a.e. z and ξ-a.e. x, we show an example below.

Consider the one-dimensional Euclidean space $\mathbb{X} = \mathbb{Z} = \mathbb{R}$ with line Borel sigma-field $\mathscr{X} = \mathscr{Z} = \mathscr{R}$ and line Lebesgue measure $\xi = \zeta = \lambda$. Let

$$\mu(\cdot|z) := \begin{cases} \delta_{z+2}, & z \in \mathbb{Q}[0,1], \\ \mathrm{Unif}[0,1], & z \in \bar{\mathbb{Q}}[0,1], \\ 0, & \text{otherwise}, \end{cases} \quad \nu(\cdot|x) := \begin{cases} \mathrm{Unif}[0,1], & x \in [0,1], \\ \delta_{x-2}, & x \in \mathbb{Q}[2,3], \\ 0, & \text{otherwise}, \end{cases} \tag{14}$$

where $\mathbb{Q}[0,1] := [0,1] \cap \mathbb{Q}$ and $\bar{\mathbb{Q}} := [0,1] \backslash \mathbb{Q}$ are the rational and irrational numbers on $[0,1]$. The conditionals are illustrated in Fig. 8. Since $\lambda(\mathbb{Q}) = 0$, the two conditionals are absolutely continuous for ζ-a.e. z and ξ-a.e. x. Consider the joint distribution on $\mathbb{X} \times \mathbb{Z} = \mathbb{R}^2$:

$$\pi := \frac{1}{2}\mathrm{Unif}([0,1] \times [0,1]) + \frac{1}{2}\sum_{z \in \mathbb{Q}[0,1]} \varrho(z)\delta_{(z+2,z)},$$

where ϱ is a distribution on the rationals $\mathbb{Q}[0,1]$ in $[0,1]$ with the sigma-field of all the subsets of $\mathbb{Q}[0,1]$. Such a distribution exists, for example, $\varrho(z) = 1/2^{n(z)}$ where $n : \mathbb{Q}[0,1] \to \mathbb{N}^*$ bijective is a numbering function of the countable set $\mathbb{Q}[0,1]$. In this way, each rational number $z \in \mathbb{Q}[0,1]$ has a positive probability, meanwhile we have $\varrho(\mathbb{Q}[0,1]) = \sum_{n=1}^{\infty} 1/2^n = 1$. Since $\pi(\{(z+2,z) \mid z \in \mathbb{Q}[0,1]\}) = \frac{1}{2}$ but $\lambda^2(\{(z+2,z) \mid z \in \mathbb{Q}[0,1]\}) = 0$ under the square Lebesgue measure λ^2, π is not absolutely continuous.

To verify compatibility, note that μ and ν here satisfy the corresponding measurability and integrability. To verify Eq. (11) reduced from Eq. (10) for defining a conditional, we first derive the marginals:

$$\pi^{\mathbb{X}} = \frac{1}{2}\mathrm{Unif}[0,1] + \frac{1}{2}\sum_{z \in \mathbb{Q}[0,1]} \varrho(z)\delta_{z+2}, \quad \pi^{\mathbb{Z}} = \frac{1}{2}\mathrm{Unif}[0,1] + \frac{1}{2}\sum_{z \in \mathbb{Q}[0,1]} \varrho(z)\delta_{z}.$$

For any $\mathcal{X} \in \mathscr{X}$ and $\mathcal{Z} \in \mathscr{Z}$, we have:

$$\begin{aligned} \pi(\mathcal{X} \times \mathcal{Z}) &= \frac{1}{2}\mathrm{Unif}[0,1](\mathcal{X})\mathrm{Unif}[0,1](\mathcal{Z}) + \frac{1}{2}\sum_{z \in \mathbb{Q}[0,1]} \varrho(z)\mathbb{I}[(z+2,z) \in \mathcal{X} \times \mathcal{Z}] \\ &= \frac{1}{2}\lambda(\mathcal{X}[0,1])\lambda(\mathcal{Z}[0,1]) + \frac{1}{2}\sum_{z \in \mathbb{Q}[0,1]} \varrho(z)\mathbb{I}[z \in (\mathcal{X} - 2) \cap \mathcal{Z}], \end{aligned}$$

where $\mathcal{X}[0,1] := [0,1] \cap \mathcal{X}$ and $\mathcal{Z}[0,1] := [0,1] \cap \mathcal{Z}$. To verify the conditional distribution $\mu(\mathcal{X}|z)$, we have:

$$\begin{aligned} \int_{\mathcal{Z}} \mu(\mathcal{X}|z)\pi^{\mathbb{Z}}(\mathrm{d}z) &= \int_{\mathcal{Z} \cap \mathbb{Q}[0,1]} \delta_{z+2}(\mathcal{X})\pi^{\mathbb{Z}}(\mathrm{d}z) + \int_{\mathcal{Z} \cap \bar{\mathbb{Q}}[0,1]} \mathrm{Unif}[0,1](\mathcal{X})\pi^{\mathbb{Z}}(\mathrm{d}z) \\ &= \int_{\mathcal{Z} \cap \mathbb{Q}[0,1]} \mathbb{I}[z+2 \in \mathcal{X}]\pi^{\mathbb{Z}}(\mathrm{d}z) + \int_{\mathcal{Z} \cap \bar{\mathbb{Q}}[0,1]} \lambda(\mathcal{X}[0,1])\pi^{\mathbb{Z}}(\mathrm{d}z) \\ &= \pi^{\mathbb{Z}}((\mathcal{X} - 2) \cap \mathcal{Z} \cap \mathbb{Q}[0,1]) + \lambda(\mathcal{X}[0,1])\pi^{\mathbb{Z}}(\mathcal{Z} \cap \bar{\mathbb{Q}}[0,1]) \end{aligned}$$

(Since a countable set has measure zero under $\mathrm{Unif}[0,1]$, *i.e.* $\lambda(\cdot \cap [0,1])$,)

$$\begin{aligned} &= \frac{1}{2}\sum_{z \in \mathbb{Q}[0,1]} \varrho(z)\mathbb{I}\big[z \in (\mathcal{X} - 2) \cap \mathcal{Z} \cap \mathbb{Q}[0,1]\big] \\ &\quad + \frac{1}{2}\lambda(\mathcal{X}[0,1])\Big(\mathrm{Unif}[0,1](\mathcal{Z}[0,1]) + \sum_{z \in \mathbb{Q}[0,1]} \varrho(z)\mathbb{I}\big[z \in \mathcal{Z} \cap \bar{\mathbb{Q}}[0,1]\big]\Big) \\ &= \frac{1}{2}\sum_{z \in \mathbb{Q}[0,1]} \varrho(z)\mathbb{I}[z \in (\mathcal{X} - 2) \cap \mathcal{Z}] + \frac{1}{2}\lambda(\mathcal{X}[0,1])\lambda(\mathcal{Z}[0,1]) = \pi(\mathcal{X} \times \mathcal{Z}). \end{aligned}$$

For the conditional distribution $\nu(\mathcal{Z}|x)$, we similarly have:

$$\begin{aligned} \int_{\mathcal{X}} \nu(\mathcal{Z}|x)\pi^{\mathbb{X}}(\mathrm{d}x) &= \int_{\mathcal{X}[0,1]} \mathrm{Unif}[0,1](\mathcal{Z})\pi^{\mathbb{X}}(\mathrm{d}x) + \int_{\mathcal{X} \cap \mathbb{Q}[2,3]} \delta_{x-2}(\mathcal{Z})\pi^{\mathbb{X}}(\mathrm{d}x) \\ &= \lambda(\mathcal{Z}[0,1])\pi^{\mathbb{X}}(\mathcal{X}[0,1]) + \pi^{\mathbb{X}}\big(\mathcal{X} \cap \mathbb{Q}[2,3] \cap (\mathcal{Z} + 2)\big) \end{aligned}$$

$$= \frac{1}{2}\lambda(\mathcal{Z}[0,1])\lambda(\mathcal{X}[0,1]) + \frac{1}{2}\sum_{z\in\mathbb{Q}[0,1]} \varrho(z)\mathbb{I}[z+2 \in \mathcal{X}\cap\mathbb{Q}[2,3]\cap(\mathcal{Z}+2)]$$
$$= \frac{1}{2}\lambda(\mathcal{Z}[0,1])\lambda(\mathcal{X}[0,1]) + \frac{1}{2}\sum_{z\in\mathbb{Q}[0,1]} \varrho(z)\mathbb{I}[z \in (\mathcal{X}-2)\cap\mathcal{Z}] = \pi(\mathcal{X}\times\mathcal{Z}).$$

So the two conditionals $\mu(\cdot|z)$ and $\nu(\cdot|x)$ are compatible and π is their joint distribution. This example illustrates that the absolute continuity of $\pi(\cdot|z)$ w.r.t ξ for ζ-a.e. z and that of $\pi(\cdot|x)$ w.r.t ζ for ξ-a.e. x, does not indicate the absolute continuity of π w.r.t $\xi\otimes\zeta$.

This example does not contradict result **(i)** of the Lemma. For any $z_0 \in \mathbb{Q}[0,1]$, we have that $\mu(\cdot|z_0) = \delta_{z_0+2}$ is not absolutely continuous w.r.t $\xi = \lambda$. But $\pi^{\mathbb{Z}}(\{z_0\}) = \frac{1}{2}\varrho(z_0) > 0$. So it is not that $\mu(\cdot|z) \ll \xi$ for $\pi^{\mathbb{Z}}$-a.e. z, which aligns with that π is not absolutely continuous w.r.t $\xi\otimes\zeta = \lambda^2$.

This example also shows that the absolute continuity of the compatible joint may depend on the joint itself, apart from the two conditionals. Consider another joint on $(\mathbb{R}^2, \mathscr{R}^2, \lambda^2)$:

$$\tilde{\pi} := \mathrm{Unif}([0,1]\times[0,1]).$$

It is easy to see that $\tilde{\pi}^{\mathbb{X}}(\mathcal{X}) = \mathrm{Unif}[0,1](\mathcal{X}) = \lambda(\mathcal{X}[0,1])$ and $\tilde{\pi}^{\mathbb{Z}}(\mathcal{Z}) = \lambda(\mathcal{Z}[0,1])$. For any $\mathcal{X} \in \mathscr{X}$ and $\mathcal{Z} \in \mathscr{Z}$, we have $\tilde{\pi}(\mathcal{X}\times\mathcal{Z}) = \lambda(\mathcal{X}[0,1])\lambda(\mathcal{Z}[0,1])$. To verify Eq. (11) for defining a conditional, we have:

$$\int_{\mathcal{Z}} \mu(\mathcal{X}|z)\tilde{\pi}^{\mathbb{Z}}(\mathrm{d}z) = \int_{\mathcal{Z}\cap\mathbb{Q}[0,1]} \delta_{z+2}(\mathcal{X})\tilde{\pi}^{\mathbb{Z}}(\mathrm{d}z) + \int_{\mathcal{Z}\cap\bar{\mathbb{Q}}[0,1]} \mathrm{Unif}[0,1](\mathcal{X})\tilde{\pi}^{\mathbb{Z}}(\mathrm{d}z)$$
$$= \int_{\mathcal{Z}\cap\mathbb{Q}[0,1]} \mathbb{I}[z+2\in\mathcal{X}]\tilde{\pi}^{\mathbb{Z}}(\mathrm{d}z) + \int_{\mathcal{Z}\cap\bar{\mathbb{Q}}[0,1]} \lambda(\mathcal{X}[0,1])\tilde{\pi}^{\mathbb{Z}}(\mathrm{d}z)$$
$$= \lambda((\mathcal{X}-2)\cap\mathcal{Z}\cap\mathbb{Q}[0,1]) + \lambda(\mathcal{X}[0,1])\lambda(\mathcal{Z}\cap\bar{\mathbb{Q}}[0,1])$$

(Since $\lambda((\mathcal{X}-2)\cap\mathcal{Z}\cap\mathbb{Q}[0,1]) \leqslant \lambda(\mathbb{Q}) = 0$ and $\lambda(\mathcal{Z}\cap\bar{\mathbb{Q}}[0,1]) = \lambda(\mathcal{Z}\cap\bar{\mathbb{Q}}[0,1]) + \lambda(\mathbb{Q}[0,1]) = \lambda(\mathcal{Z}[0,1])$,)

$$= \lambda(\mathcal{X}[0,1])\lambda(\mathcal{Z}[0,1]) = \tilde{\pi}(\mathcal{X}\times\mathcal{Z}).$$

For the conditional distribution $\nu(\mathcal{Z}|x)$, we similarly have:

$$\int_{\mathcal{X}} \nu(\mathcal{Z}|x)\tilde{\pi}^{\mathbb{X}}(\mathrm{d}x) = \int_{\mathcal{X}[0,1]} \mathrm{Unif}[0,1](\mathcal{Z})\tilde{\pi}^{\mathbb{X}}(\mathrm{d}x) + \int_{\mathcal{X}\cap\mathbb{Q}[2,3]} \delta_{x-2}(\mathcal{Z})\tilde{\pi}^{\mathbb{X}}(\mathrm{d}x)$$
$$= \lambda(\mathcal{Z}[0,1])\tilde{\pi}^{\mathbb{X}}(\mathcal{X}[0,1]) + \tilde{\pi}^{\mathbb{X}}\big(\mathcal{X}\cap\mathbb{Q}[2,3]\cap(\mathcal{Z}+2)\big)$$

(Since $\tilde{\pi}^{\mathbb{X}}\big(\mathcal{X}\cap\mathbb{Q}[2,3]\cap(\mathcal{Z}+2)\big) = \lambda\big(\mathcal{X}\cap\mathbb{Q}[2,3]\cap(\mathcal{Z}+2)\cap[0,1]\big) \leqslant \lambda(\mathbb{Q}) = 0$,)

$$= \lambda(\mathcal{Z}[0,1])\lambda(\mathcal{X}[0,1]) = \tilde{\pi}(\mathcal{X}\times\mathcal{Z}).$$

So $\tilde{\pi}$ is also a compatible joint of $\mu(\cdot|z)$ and $\nu(\cdot|x)$. In this case, the violation set for $\mu(\cdot|z) \ll \xi$, *i.e.* $\mathbb{Q}[0,1]$, has measure zero under $\tilde{\pi}^{\mathbb{Z}}$, and the violation set for $\nu(\cdot|x) \ll \zeta$, *i.e.* $\mathbb{Q}[2,3]$, has measure zero under $\tilde{\pi}^{\mathbb{X}}$. So result **(i)** of the Lemma asserts that $\tilde{\pi} \ll \xi\otimes\zeta$, which aligns with the example. This example shows that although both π and $\tilde{\pi}$ are the compatible joint of the same conditionals, they have different absolute continuity. So the condition in result **(i)** of the Lemma requires the knowledge of the marginals $\pi^{\mathbb{Z}}$ and $\pi^{\mathbb{X}}$.

C.2 Proof of Theorem 2.3

Example C.3. Before presenting the proof, we give an example showing that only being the intersection of $\mathcal{W}_{p,q}$ and $\mathcal{W}_{q,p}$ is not sufficient to make a valid support of a compatible joint. The example is illustrated in Fig. 9. The conditionals are uniform on the respective depicted slices, so conditions **(iv)** and **(v)** in the theorem (2.3) are satisfied. The sets $\mathcal{W}_{p,q}$ and $\mathcal{W}_{q,p}$ are depicted in the figure, and their intersection $\mathcal{W}_{p,q}\cap\mathcal{W}_{q,p}$ is the right half. Although on $\mathcal{W}_{p,q}\cap\mathcal{W}_{q,p}$, the conditionals do not render support conflict, the conditional $q(z|x)$ is unnormalized for a given x from the bottom half: it integrates to $1/2$ on $(\mathcal{W}_{p,q}\cap\mathcal{W}_{q,p})_x$. This means

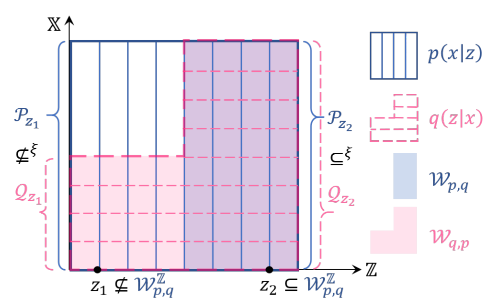


Figure 9: Illustration of Example C.3. The conditionals are uniform on the respective depicted slices. On $\mathcal{W}_{p,q}\cap\mathcal{W}_{q,p}$, the conditional $q(z|x)$ is not normalized.

that any compatible joint π would also have its conditional $\pi(\cdot|x)$ unnormalized for such x, which is impossible.

One may consider trying $\mathcal{W}_{q,p}$ as the joint support. This renders a support conflict similar to the example in the main text: a joint on $\mathcal{W}_{q,p}$ is required by $p(x|z)$ to also cover the top-left quadrant since z values in the left half are covered, but this contradicts with the absence of mass by $q(z|x)$. In fact, in this example, there is no $\xi\otimes\zeta$-complete component of both $\mathcal{W}_{p,q}$ and $\mathcal{W}_{q,p}$, so the two conditionals are not compatible.

***Proof*.** Let $\mu(\mathcal{X}|z)$ and $\nu(\mathcal{Z}|x)$ be the two everywhere absolutely continuous conditional distributions of whom $p(x|z)$ and $q(z|x)$ are the density functions. We begin with some useful conclusions.

(1) By construction, for any $(x,z) \in \mathcal{W}_{p,q}$, $p(x|z) > 0$. For any $z \in \mathcal{W}_{p,q}^{\mathbb{Z}}$, we have $\xi\{x \in (\mathcal{W}_{p,q})_z \mid q(z|x) = 0\} = \xi\{x \in \mathcal{P}_z \mid x \notin \mathcal{Q}_z\} = \xi(\mathcal{P}_z \setminus \mathcal{Q}_z) = 0$, which means that $q(z|x) > 0$, ξ-a.e. on $(\mathcal{W}_{p,q})_z$. By Lemma B.10, we have that $q(z|x) > 0$, $\xi\otimes\zeta$-a.e. on $\mathcal{W}_{p,q}$. Symmetrically, $q(z|x) > 0$ on $\mathcal{W}_{q,p}$, and $p(x|z) > 0$, $\xi\otimes\zeta$-a.e. on $\mathcal{W}_{q,p}$. Particularly, the ratio $\frac{p(x|z)}{q(z|x)}$ is well-defined and is positive and finite, both $\xi\otimes\zeta$-a.e. on $\mathcal{W}_{p,q}$ and $\xi\otimes\zeta$-a.e. on $\mathcal{W}_{q,p}$. The conclusions also hold ($\xi\otimes\zeta$-a.e.) on any ($\xi\otimes\zeta$-a.s.) subset of $\mathcal{W}_{p,q}$ or $\mathcal{W}_{q,p}$.

"Only if" (necessity):

Let π be a compatible joint distribution of such conditional distributions $\mu(\cdot|z)$ and $\nu(\cdot|x)$.

(2) Since "for any" indicates "a.e." under any measure, the conditions in Lemma C.1 are satisfied, so we have $\pi \ll \xi\otimes\zeta$. By Lemma B.9, we also have $\pi^{\mathbb{X}} \ll \xi$ and $\pi^{\mathbb{Z}} \ll \zeta$. So there exist density functions (R-N derivatives; 9, Thm. 32.2) $u(x)$ and $v(z)$ such that for any $\mathcal{X} \in \mathscr{X}$ and $\mathcal{Z} \in \mathscr{Z}$, $\pi^{\mathbb{X}}(\mathcal{X}) = \int_{\mathcal{X}} u(x)\xi(\mathrm{d}x)$ and $\pi^{\mathbb{Z}}(\mathcal{Z}) = \int_{\mathcal{Z}} v(z)\zeta(\mathrm{d}z)$. This $u(x)$ is obviously ξ-integrable on any measurable subset of $\mathbb{X}$, since the integral is no larger (since u is nonnegative) than $\int_{\mathbb{X}} u(x)\xi(\mathrm{d}x) = 1$ which is finite.

(3) By the definition of conditional distribution Eq. (11), for any $\mathcal{X}\times\mathcal{Z} \in \mathscr{X}\times\mathscr{Z}$, we have $\pi(\mathcal{X}\times\mathcal{Z}) = \int_{\mathcal{Z}} \mu(\mathcal{X}|z)\pi^{\mathbb{Z}}(\mathrm{d}z) = \int_{\mathcal{Z}} \mu(\mathcal{X}|z)v(z)\zeta(\mathrm{d}z) = \int_{\mathcal{Z}}\int_{\mathcal{X}} p(x|z)\xi(\mathrm{d}x)v(z)\zeta(\mathrm{d}z) = \int_{\mathcal{X}\times\mathcal{Z}} p(x|z)v(z)(\xi\otimes\zeta)(\mathrm{d}x\mathrm{d}z)$, where in the last equality, we have applied Fubini's theorem Eq. (8) [9, Thm. 18.3]. Similarly, $\pi(\mathcal{X}\times\mathcal{Z}) = \int_{\mathcal{X}\times\mathcal{Z}} q(z|x)u(x)(\xi\otimes\zeta)(\mathrm{d}x\mathrm{d}z)$. Noting that $\mathscr{X}\times\mathscr{Z}$ is the pi-system that generates $\mathscr{X}\otimes\mathscr{Z}$, this indicates that $p(x|z)v(z) = q(z|x)u(x)$, $\xi\otimes\zeta$-a.e. on $\mathbb{X}\times\mathbb{Z}$ [9, Thm. 16.10(iii)][10]. In other words, both $p(x|z)v(z)$ and $q(z|x)u(x)$ are density functions of π.
(3.1) Subsequently, by leveraging Lemma B.10, we have for ζ-a.e. z on $\mathbb{Z}$, $p(x|z)v(z) = q(z|x)u(x)$, ξ-a.e. on $\mathbb{X}$.

(4) Let $\mathcal{U} := \{x \mid u(x) > 0\}$ and $\mathcal{V} := \{z \mid v(z) > 0\}$, and define:

$$\mathcal{S} := (\mathcal{U}\times\mathcal{V}) \cap \mathcal{W}_{p,q}, \quad \tilde{\mathcal{S}} := (\mathcal{U}\times\mathcal{V}) \cap \mathcal{W}_{q,p}, \tag{15}$$

Since u and v are integrable thus measurable and $\mathbb{R}^{>0}$ is Lebesgue-measurable, we know that $\mathcal{U} \in \mathscr{X}$ and $\mathcal{V} \in \mathscr{Z}$ are also measurable. So $\mathcal{S}$ and $\tilde{\mathcal{S}}$ are measurable.

(4.1) We can verify that $\mathcal{S}$ is a $\xi\otimes\zeta$-complete component of $\mathcal{W}_{p,q}$. Since $\mathcal{S} \subseteq \mathcal{W}_{p,q}$, we only need to verify that:

$$(\xi\otimes\zeta)\big([(\mathcal{S}^{\mathbb{X}}\times\mathbb{Z} \cup \mathbb{X}\times\mathcal{S}^{\mathbb{Z}}) \cap \mathcal{W}_{p,q}] \setminus \mathcal{S}\big)$$

(Since clearly $\mathcal{S}^{\mathbb{X}} \subseteq \mathcal{U}$, $\mathcal{S}^{\mathbb{Z}} \subseteq \mathcal{V}$, and measures are monotone,)

$$\leqslant (\xi\otimes\zeta)\big([(\mathcal{U}\times\mathbb{Z} \cup \mathbb{X}\times\mathcal{V}) \cap \mathcal{W}_{p,q}] \setminus \mathcal{S}\big) \qquad \text{(Since } (\mathcal{A}\cap\mathcal{C}) \setminus (\mathcal{B}\cap\mathcal{C}) = (\mathcal{A}\setminus\mathcal{B}) \cap \mathcal{C}\text{,)}$$

$$= (\xi\otimes\zeta)\big([(\mathcal{U}\times\mathbb{Z} \cup \mathbb{X}\times\mathcal{V}) \setminus (\mathcal{U}\times\mathcal{V})] \cap \mathcal{W}_{p,q}\big) \qquad \text{(Since } (\mathcal{A}\cup\mathcal{B}) \setminus \mathcal{C} = (\mathcal{A}\setminus\mathcal{C}) \cup (\mathcal{B}\setminus\mathcal{C})\text{,)}$$

$$= (\xi\otimes\zeta)\big([((\mathcal{U}\times\mathbb{Z}) \setminus (\mathcal{U}\times\mathcal{V})) \cup ((\mathbb{X}\times\mathcal{V}) \setminus (\mathcal{U}\times\mathcal{V}))] \cap \mathcal{W}_{p,q}\big)$$

$$= (\xi\otimes\zeta)\big([\{(x,z) \mid u(x) > 0, v(z) = 0\} \cup \mathcal{W}_{p,q}] \cup [\{(x,z) \mid u(x) = 0, v(z) > 0\} \cup \mathcal{W}_{p,q}]\big)$$

[10] The requirement that $\mathbb{X}\times\mathbb{Z}$ is a finite or countable union of $\mathscr{X}\times\mathscr{Z}$-sets is satisfied, since from the sigma-finiteness of ξ and ζ, $\mathbb{X}$ and $\mathbb{Z}$ are a finite or countable union of (ξ-finite) $\mathscr{X}$-sets and (ζ-finite) $\mathscr{Z}$-sets, respectively.

(By Conclusion **(3)** and adjusting the set by a set of $\xi\otimes\zeta$-measure-zero according to Lemma B.1,)

$= (\xi\otimes\zeta)\big(\big[\{(x,z) \mid u(x)>0, v(z)=0, q(z|x)=0\} \cup \mathcal{W}_{p,q}\big]$
$\quad \cup \big[\{(x,z) \mid u(x)=0, v(z)>0, p(x|z)=0\} \cup \mathcal{W}_{p,q}\big]\big)$
$\leqslant (\xi\otimes\zeta)\big(\{(x,z) \mid u(x)>0, v(z)=0, q(z|x)=0\} \cup \mathcal{W}_{p,q}\big)$
$\quad + (\xi\otimes\zeta)\big(\{(x,z) \mid u(x)=0, v(z)>0, p(x|z)=0\} \cup \mathcal{W}_{p,q}\big)$ (By Conclusion **(1)**,)
$= 0$. Symmetrically, we can also verify that $\tilde{\mathcal{S}}$ is a $\xi\otimes\zeta$-complete component of $\mathcal{W}_{q,p}$.

(4.2) We can also show that $\pi(\mathcal{S}) = \pi(\tilde{\mathcal{S}}) = 1$. From Conclusion **(3)**, we have:

$1 = \pi(\mathbb{X}\times\mathbb{Z}) = \int_{\mathbb{Z}}\int_{\mathbb{X}} p(x|z)\xi(\mathrm{d}x)v(z)\zeta(\mathrm{d}z)$

(Since the integral on a region with an a.e. zero value is zero [9, Thm. 15.2(i)],)

$= \int_{\mathcal{V}}\int_{\mathcal{P}_z} p(x|z)\xi(\mathrm{d}x)v(z)\zeta(\mathrm{d}z)$ (Since $\mathcal{S}^{\mathbb{Z}} \subseteq \mathcal{V}$ and due to Billingsley [9, Thm. 16.9],)

$= \Big(\int_{\mathcal{S}^{\mathbb{Z}}}\int_{\mathcal{P}_z} + \int_{\mathcal{V}\setminus\mathcal{S}^{\mathbb{Z}}}\int_{\mathcal{P}_z}\Big) p(x|z)\xi(\mathrm{d}x)v(z)\zeta(\mathrm{d}z)$ (Since $\mathcal{V}\setminus\mathcal{S}^{\mathbb{Z}} = \mathcal{V}\setminus(\mathcal{V}\cap\mathcal{W}^{\mathbb{Z}}_{p,q}) = \mathcal{V}\setminus\mathcal{W}^{\mathbb{Z}}_{p,q}$,)

$= \Big(\int_{\mathcal{S}^{\mathbb{Z}}}\int_{\mathcal{P}_z} + \int_{\mathcal{V}\setminus\mathcal{W}^{\mathbb{Z}}_{p,q}}\int_{\mathcal{P}_z}\Big) p(x|z)\xi(\mathrm{d}x)v(z)\zeta(\mathrm{d}z).$

For the second iterated integral, note that for any z on $\mathcal{V}$, $v(z)>0$, so from Conclusion **(3.1)**, for ζ-a.e. z on $\mathcal{V}$, we have $p(x|z)>0 \Longrightarrow q(z|x)>0$, ξ-a.e. on $\mathbb{X}$. This means that for ζ-a.e. z on $\mathcal{V}$, $\xi\{x \mid p(x|z)>0, q(z|x)=0\} = \xi(\mathcal{P}_z\setminus\mathcal{Q}_z) = 0$. So the set $\mathcal{V}\setminus\mathcal{W}^{\mathbb{Z}}_{p,q} = \{z\in\mathcal{V} \mid \xi(\mathcal{P}_z\setminus\mathcal{Q}_z)>0 \text{ or } \mathcal{P}_z=\emptyset\}$ has the same measure under ζ as the set $\{z\in\mathcal{V} \mid \mathcal{P}_z=\emptyset\}$. This means that the second iterated integral $\int_{\mathcal{V}\setminus\mathcal{W}^{\mathbb{Z}}_{p,q}}\int_{\mathcal{P}_z} p(x|z)\xi(\mathrm{d}x)v(z)\zeta(\mathrm{d}z) = \int_{\{z\in\mathcal{V}\mid\mathcal{P}_z=\emptyset\}}\int_{\mathcal{P}_z} p(x|z)\xi(\mathrm{d}x)v(z)\zeta(\mathrm{d}z) = 0$ [9, p.226, Thm. 15.2(i)].

For the first iterated integral, note that by construction, $\mathcal{P}_z = (\mathcal{W}_{p,q})_z$ for any z on $\mathcal{S}^{\mathbb{Z}}$, since $\mathcal{S}^{\mathbb{Z}} \subseteq \mathcal{W}^{\mathbb{Z}}_{p,q}$. Moreover, from Conclusion **(4.1)** that $\mathcal{S}$ is a $\xi\otimes\zeta$-complete component of $\mathcal{W}_{p,q}$, we can subsequently apply Lemma B.16, so $\int_{\mathcal{S}^{\mathbb{Z}}}\int_{(\mathcal{W}_{p,q})_z} p(x|z)\xi(\mathrm{d}x)v(z)\zeta(\mathrm{d}z) = \int_{\mathcal{S}} p(x|z)v(z)(\xi\otimes\zeta)(\mathrm{d}x\mathrm{d}z)$, which is $\pi(\mathcal{S})$ by Conclusion **(3)**. This means that $\pi(\mathcal{S})=1$. The same deduction applies symmetrically to $\tilde{\mathcal{S}}$, so we also have $\pi(\tilde{\mathcal{S}})=1$.

Main procedure ("only if"). We will verify that the set $\mathcal{S}$ given in Eq. (15) satisfies all the necessary conditions.

Conclusion **(4.2)** shows that $\pi(\mathcal{S}) = 1 > 0$, and in Conclusion **(2)** we have verified that $\pi \ll \xi\otimes\zeta$. So we have $(\xi\otimes\zeta)(\mathcal{S}) > 0$, which verifies Condition **(iii)**.

To verify Conditions **(iv)** and **(v)**, by Conclusions **(3)** and **(1)**, we have $p(x|z)v(z) = q(z|x)u(x)$ and $q(z|x)>0$, $\xi\otimes\zeta$-a.e. on $\mathcal{S}$. By the construction of $\mathcal{S}$, we also have $v(z)>0$ and $p(x|z)>0$ everywhere on $\mathcal{S}$. So the ratio $\frac{p(x|z)}{q(z|x)}$ is finite and positive, $\xi\otimes\zeta$-a.e. on $\mathcal{S}$, and it factorizes as $\frac{p(x|z)}{q(z|x)} = u(x)\frac{1}{v(z)}$, $\xi\otimes\zeta$-a.e. on $\mathcal{S}$. By Conclusion **(2)**, $a(x) := u(x)$ is ξ-integrable on $\mathcal{S}^{\mathbb{X}}$.

To verify Condition **(ii)**, note that by construction, $\mathcal{S}^{\mathbb{Z}} \subseteq \mathcal{V}\cap\mathcal{W}^{\mathbb{Z}}_{p,q} \subseteq \mathcal{W}^{\mathbb{Z}}_{p,q}$ so $\mathcal{S}^{\mathbb{Z}} \subseteq^{\zeta} \mathcal{W}^{\mathbb{Z}}_{p,q}$. Note that $\mathcal{S}^{\mathbb{X}} = \{x\in\mathcal{U} \mid \mathcal{V}\cap(\mathcal{W}_{p,q})_x \neq \emptyset\} = \{x\in\mathcal{U} \mid \exists z\in\mathcal{V} \text{ s.t. } x\in\mathcal{P}_z, \mathcal{P}_z \subseteq^{\xi} \mathcal{Q}_z\} \subseteq \{x\in\mathcal{U} \mid \exists z\in\mathcal{V} \text{ s.t. } x\in\mathcal{P}_z\} = \{x \mid u(x)>0, \exists z \text{ s.t. } v(z)>0, p(x|z)>0\}$. By Conclusion **(3.1)**, for ξ-a.e. x on $\mathcal{S}^{\mathbb{X}}$, we have $\exists z$ s.t. $q(z|x)u(x) = p(x|z)v(z) > 0$, so $q(z|x)>0$ hence $\mathcal{Q}_x \neq \emptyset$. Moreover, for ξ-a.e. x on $\mathcal{S}^{\mathbb{X}}$ and ζ-a.e. z on $\mathcal{Q}_x$, we have $p(x|z)v(z) = q(z|x)u(x) > 0$, so $p(x|z)>0$ hence $\mathcal{Q}_x \subseteq^{\zeta} \mathcal{P}_x$. These two conclusions means that for ξ-a.e. x on $\mathcal{S}^{\mathbb{X}}$, we have $x \in \{x \mid \mathcal{Q}_x \neq \emptyset, \mathcal{Q}_x \subseteq^{\zeta} \mathcal{P}_x\}$ which is exactly $\mathcal{W}^{\mathbb{X}}_{q,p}$. Hence $\mathcal{S}^{\mathbb{X}} \subseteq^{\xi} \mathcal{W}^{\mathbb{X}}_{q,p}$.

Now, all the left is to verify Condition **(i)**. Conclusion **(4.1)** has verified that $\mathcal{S}$ is a $\xi\otimes\zeta$-complete component of $\mathcal{W}_{p,q}$. To verify that $\mathcal{S}$ is a $\xi\otimes\zeta$-complete component also of $\mathcal{W}_{q,p}$, note that Conclusion **(4.1)** has also verified that $\tilde{\mathcal{S}}$ is a $\xi\otimes\zeta$-complete component of $\mathcal{W}_{q,p}$, so by Lemma B.14 it suffices to verify that $\mathcal{S} \overset{\xi\otimes\zeta}{=} \tilde{\mathcal{S}}$, $\mathcal{S}^{\mathbb{X}} \overset{\xi}{=} \tilde{\mathcal{S}}^{\mathbb{X}}$ and $\mathcal{S}^{\mathbb{Z}} \overset{\zeta}{=} \tilde{\mathcal{S}}^{\mathbb{Z}}$.

By construction, for any $(x,z) \in \mathcal{S}$, we have $v(z) > 0$ and $p(x|z) > 0$, so from Conclusion **(3)** the density function $p(x|z)v(z)$ of π is positive. Similarly, the density function $q(z|x)u(x)$ of π is positive everywhere on $\tilde{\mathcal{S}}$. Moreover, Conclusion **(4.2)** has shown that both $\pi(\mathcal{S}) = 1$ and $\pi(\tilde{\mathcal{S}}) = 1$. So by Lemma B.7, we know that $\mathcal{S} \overset{\xi\otimes\zeta}{=} \tilde{\mathcal{S}}$. Also by construction, the density function $u(x)$ of $\pi^{\mathbb{X}}$ is positive everywhere on $\mathcal{S}^{\mathbb{X}}$ and on $\tilde{\mathcal{S}}^{\mathbb{X}}$. Moreover, we have $\pi^{\mathbb{X}}(\mathcal{S}^{\mathbb{X}}) = \pi(\mathcal{S}^{\mathbb{X}} \times \mathbb{Z}) \geqslant \pi(\mathcal{S}) = 1$ so $\pi^{\mathbb{X}}(\mathcal{S}^{\mathbb{X}}) = 1$ and similarly $\pi^{\mathbb{X}}(\tilde{\mathcal{S}}^{\mathbb{X}}) = 1$. Again by Lemma B.7, we have $\mathcal{S}^{\mathbb{X}} \overset{\xi}{=} \tilde{\mathcal{S}}^{\mathbb{X}}$. It follows similarly that $\mathcal{S}^{\mathbb{Z}} \overset{\zeta}{=} \tilde{\mathcal{S}}^{\mathbb{Z}}$.

"If" (sufficiency):

(5) For Conditions **(iv)** and **(v)**, denote $\tilde{a}(x) := |a(x)|$ and $\tilde{b}(z) := |b(z)|$, and let $\tilde{A} := \int_{\mathcal{S}^{\mathbb{X}}} \tilde{a}(x)\xi(\mathrm{d}x)$.
(5.1) From the definition of integrability in Supplement A.1, Condition **(v)** is equivalent to that $\tilde{a}(x)$ is ξ-integrable on $\mathcal{S}^{\mathbb{X}}$. Particularly, $\tilde{A} < \infty$.
Due to Condition **(i)** and Lemma B.12, we have $\mathcal{S} \subseteq^{\xi\otimes\zeta} \mathcal{W}_{p,q}$. So by Condition **(iv)** and Conclusion **(1)**, we have $\frac{p(x|z)}{q(z|x)} = a(x)b(z) > 0$, $\xi\otimes\zeta$-a.e. on $\mathcal{S}$. This means both $(\xi\otimes\zeta)\{(x,z) \in \mathcal{S} \mid a(x)b(z) = 0\} = 0$ and $(\xi\otimes\zeta)\{(x,z) \in \mathcal{S} \mid a(x)b(z) < 0\} = 0$, since their summation is zero.
(5.2) Since $\{(x,z) \mid x \in \mathcal{S}^{\mathbb{X}}, a(x) = 0, z \in \mathcal{S}_x\} \subseteq \{(x,z) \in \mathcal{S} \mid a(x)b(z) = 0\}$, the second-last equation in Conclusion **(5.1)** above means that $(\xi\otimes\zeta)\{(x,z) \mid x \in \mathcal{S}^{\mathbb{X}}, a(x) = 0, z \in \mathcal{S}_x\} = 0$. So $(\xi\otimes\zeta)\{(x,z) \mid x \in \mathcal{S}^{\mathbb{X}}, a(x) \neq 0, z \in \mathcal{S}_x\} = (\xi\otimes\zeta)\{(x,z) \mid x \in \mathcal{S}^{\mathbb{X}}, z \in \mathcal{S}_x\} - (\xi\otimes\zeta)\{(x,z) \mid x \in \mathcal{S}^{\mathbb{X}}, a(x) = 0, z \in \mathcal{S}_x\} = (\xi\otimes\zeta)(\mathcal{S}) > 0$ by Condition **(iii)**. Moreover, by Eq. (7), we have $(\xi\otimes\zeta)\{(x,z) \mid x \in \mathcal{S}^{\mathbb{X}}, a(x) \neq 0, z \in \mathcal{S}_x\} = \int_{\{x \in \mathcal{S}^{\mathbb{X}} \mid a(x) \neq 0\}} \zeta(\mathcal{S}_x)\xi(\mathrm{d}x) > 0$, so $\xi\{x \in \mathcal{S}^{\mathbb{X}} \mid a(x) \neq 0\} > 0$ [9, p.226]. Particularly, $\tilde{A} > 0$ [9, Thm. 15.2(ii)].
(5.3) Since $\{(x,z) \in \mathcal{S} \mid a(x)b(z) \neq \tilde{a}(x)\tilde{b}(z)\} = \{(x,z) \in \mathcal{S} \mid a(x)b(z) < 0\}$, the last equation in Conclusion **(5.1)** above means that $a(x)b(z) = \tilde{a}(x)\tilde{b}(z)$, $\xi\otimes\zeta$-a.e. on $\mathcal{S}$. So we have $\frac{p(x|z)}{q(z|x)} = \tilde{a}(x)\tilde{b}(z)$, $\xi\otimes\zeta$-a.e. on $\mathcal{S}$, following Condition **(iv)**.

(6) Based on Conclusions **(5.1)** and **(5.2)**, we can define the following finite and nonnegative functions on $\mathbb{X}$ and $\mathbb{Z}$:

$$u(x) := \begin{cases} \frac{1}{\tilde{A}}\tilde{a}(x), & \text{if } x \in \mathcal{S}^{\mathbb{X}} \text{ and } \tilde{a}(x) > 0, \\ 0, & \text{otherwise,} \end{cases} \qquad v(z) := \begin{cases} \frac{1}{\tilde{A}\tilde{b}(z)}, & \text{if } z \in \mathcal{S}^{\mathbb{Z}} \text{ and } \tilde{b}(z) > 0, \\ 0, & \text{otherwise.} \end{cases}$$

(6.1) By construction, $\tilde{a}(x)\tilde{b}(z) = u(x)/v(z)$ on $\mathcal{S} \cap \{(x,z) \mid \tilde{b}(z) > 0\}$. So from Conclusion **(5.3)**, we have $p(x|z)v(z) = q(z|x)u(x)$, $\xi\otimes\zeta$-a.e. on $\mathcal{S} \cap \{(x,z) \mid \tilde{b}(z) > 0\}$. Moreover, following a similar deduction as in Conclusion **(5.2)**, we know that $(\xi\otimes\zeta)(\mathcal{S} \setminus \{(x,z) \mid \tilde{b}(z) > 0\}) = (\xi\otimes\zeta)\{(x,z) \mid z \in \mathcal{S}^{\mathbb{Z}}, b(z) = 0, x \in \mathcal{S}_z\} = 0$. So we have $p(x|z)v(z) = q(z|x)u(x)$, $\xi\otimes\zeta$-a.e. on $\mathcal{S}$.
(6.2) By construction, $\int_{\mathbb{X}} u(x)\xi(\mathrm{d}x) = \int_{\mathcal{S}^{\mathbb{X}}} u(x)\xi(\mathrm{d}x) = 1$.

Main procedure ("if"). We will show that the following function on $\mathscr{X} \otimes \mathscr{Z}$, which is the same as Eq. (1) in the theorem, is a distribution on $\mathbb{X} \times \mathbb{Z}$ such that $\mu(\mathcal{X}|z)$ and $\nu(\mathcal{Z}|x)$ are its conditional distributions:

$$\pi(\mathcal{W}) := \int_{\mathcal{W}\cap\mathcal{S}} q(z|x)u(x)(\xi\otimes\zeta)(\mathrm{d}x\mathrm{d}z), \quad \forall \mathcal{W} \in \mathscr{X} \otimes \mathscr{Z}. \tag{16}$$

Consider any measurable rectangle $\mathcal{X} \times \mathcal{Z} \in \mathscr{X} \times \mathscr{Z}$. We have:

$$\pi(\mathcal{X} \times \mathcal{Z}) = \int_{\mathcal{X}\times\mathcal{Z}\cap\mathcal{S}} q(z|x)u(x)(\xi\otimes\zeta)(\mathrm{d}x\mathrm{d}z)$$

(By the generalized form Eq. (9) of Fubini's theorem,)

$$= \int_{\mathcal{X}\cap\mathcal{S}^{\mathbb{X}}} \int_{\mathcal{Z}\cap\mathcal{S}_x} q(z|x)\zeta(\mathrm{d}z)u(x)\xi(\mathrm{d}x)$$

(By Condition **(i)** and applying Lemma B.16,)

$$= \int_{\mathcal{X}\cap\mathcal{S}^{\mathbb{X}}} \int_{\mathcal{Z}\cap(\mathcal{W}_{q,p})_x} q(z|x)\zeta(\mathrm{d}z)u(x)\xi(\mathrm{d}x)$$

(Since $\mathcal{S}^{\mathbb{X}} \subseteq^{\xi} \mathcal{W}_{q,p}^{\mathbb{X}}$ by Condition **(ii)** and $(\mathcal{W}_{q,p})_x = \mathcal{Q}_x$ on $\mathcal{W}_{q,p}^{\mathbb{X}}$,)

$$= \int_{\mathcal{X}\cap\mathcal{S}^{\mathbb{X}}} \int_{\mathcal{Z}\cap\mathcal{Q}_x} q(z|x)\zeta(\mathrm{d}z)u(x)\xi(\mathrm{d}x)$$

(Since by construction, $u(x) = 0$ outside $\mathcal{S}^{\mathbb{X}}$ and $q(z|x) = 0$ outside $\mathcal{Q}_x$,)

$$= \int_{\mathcal{X}} \int_{\mathcal{Z}} q(z|x)\zeta(\mathrm{d}z)u(x)\xi(\mathrm{d}x) \qquad \text{(Recalling that } q(z|x) \text{ is the density function of } \nu(\cdot|x),)$$

$$= \int_{\mathcal{X}} \nu(\mathcal{Z}|x)u(x)\xi(\mathrm{d}x). \tag{17}$$

Moreover, due to Conclusion **(6.1)**, we have $\pi(\mathcal{W}) = \int_{\mathcal{W}\cap\mathcal{S}} p(x|z)v(z)(\xi\otimes\zeta)(\mathrm{d}x\mathrm{d}z)$ on $\mathscr{X}\otimes\mathscr{Z}$ [9, Thm. 15.2(v)]. Using this form of π and noting that the symmetrized conditions in the above deduction also hold, we have:

$$\pi(\mathcal{X}\times\mathcal{Z}) = \int_{\mathcal{Z}} \mu(\mathcal{X}|z)v(z)\zeta(\mathrm{d}z). \tag{18}$$

Since both $q(z|x)$ and $u(x)$ are finite and nonnegative on $\mathbb{X}\times\mathbb{Z}$, π is a measure on $\mathscr{X}\otimes\mathscr{Z}$ by its definition Eq. (16) [9, p.227]. Moreover, from Eq. (17), we have $\pi(\mathbb{X}\times\mathbb{Z}) = \int_{\mathbb{X}} u(x)\xi(\mathrm{d}x) = 1$ by Conclusion **(6.2)**. So π is a distribution (probability measure) on $\mathbb{X}\times\mathbb{Z}$.

From Eq. (17), we have $\pi^{\mathbb{X}}(\mathcal{X}) := \pi(\mathcal{X}\times\mathbb{Z}) = \int_{\mathcal{X}} u(x)\xi(\mathrm{d}x)$. So $u(x)$ is a density function of $\pi^{\mathbb{X}}$, and Eq. (17) in turn becomes $\pi(\mathcal{X}\times\mathcal{Z}) = \int_{\mathcal{X}} \nu(\mathcal{Z}|x)\pi^{\mathbb{X}}(\mathrm{d}x)$. This indicates that $\nu(\mathcal{Z}|x)$ is a conditional distribution of π w.r.t sub-sigma-field $\mathscr{X}\times\{\mathcal{Z}\}$ for any $\mathcal{Z}\in\mathscr{Z}$, due to Eq. (11).

Similarly, from Eq. (18), we have $\pi^{\mathbb{Z}}(\mathcal{Z}) := \pi(\mathbb{X}\times\mathcal{Z}) = \int_{\mathcal{Z}} v(z)\zeta(\mathrm{d}z)$. So $v(z)$ is a density function of $\pi^{\mathbb{Z}}$, and Eq. (18) in turn becomes $\pi(\mathcal{X}\times\mathcal{Z}) = \int_{\mathcal{Z}} \mu(\mathcal{X}|z)\pi^{\mathbb{Z}}(\mathrm{d}z)$. This indicates that $\mu(\mathcal{X}|z)$ is a conditional distribution of π w.r.t sub-sigma-field $\{\mathcal{X}\}\times\mathscr{Z}$ for any $\mathcal{X}\in\mathscr{X}$, due to Eq. (11). The proof is completed. □

C.3 Complete Support Proposition under the a.e.-Full Support Condition

Proposition C.4. *If $p(x|z)$ and $q(z|x)$ have a.e.-full supports, then $\mathcal{W}_{p,q} \overset{\xi\otimes\zeta}{=} \mathcal{W}_{q,p} \overset{\xi\otimes\zeta}{=} \mathbb{X}\times\mathbb{Z}$, and $\mathbb{X}\times\mathbb{Z}$ is the $\xi\otimes\zeta$-unique complete support of them when compatible.*

Proof. By definition, $p(x|z) > 0$ and $q(z|x) > 0$, $\xi\otimes\zeta$-a.e. By Lemma B.10, this means that for ξ-a.e. x, $p(x|z) > 0$ ζ-a.e. thus $\mathcal{P}_x \overset{\zeta}{=} \mathbb{Z}$, and for ζ-a.e. z, $\mathcal{Q}_z \overset{\xi}{=} \mathbb{X}$. Similarly, we also have for ξ-a.e. x, $\mathcal{Q}_x \overset{\zeta}{=} \mathbb{Z}$ thus $\mathcal{Q}_x \overset{\zeta}{=} \mathcal{P}_x$ by the transitivity (Lemma B.4) and subsequently $\mathcal{Q}_x \subseteq^{\zeta} \mathcal{P}_x$. Similarly, for ζ-a.e. z, $\mathcal{P}_z \subseteq^{\xi} \mathcal{Q}_z$. This means that for ξ-a.e. x, $(\mathcal{W}_{q,p})_x = \mathcal{Q}_x \overset{\zeta}{=} \mathbb{Z}$ thus $z \in (\mathcal{W}_{q,p})_x$, ζ-a.e. By Lemma B.10, this means that for $\xi\otimes\zeta$-a.e. (x,z), we have $(x,z)\in\mathcal{W}_{q,p}$, so $\mathcal{W}_{q,p} \overset{\xi\otimes\zeta}{=} \mathbb{X}\times\mathbb{Z}$. Similarly, we have $\mathcal{W}_{p,q} \overset{\xi\otimes\zeta}{=} \mathbb{X}\times\mathbb{Z}$.

Let $\mathcal{S}$ be a complete support of $p(x|z)$ and $q(z|x)$ when they are compatible. Since $(\xi\otimes\zeta)(\mathcal{S}) = 1 > 0$ from Condition **(iii)** in Theorem 2.3, we know that $\xi(\mathcal{S}^{\mathbb{X}}) > 0$ by Eq. (7) and Billingsley [9, p.226]. So there is an $x\in\mathcal{S}^{\mathbb{X}}$ such that $(\mathcal{W}_{q,p})_x \overset{\zeta}{=} \mathbb{Z}$, otherwise there would be a non-measure-zero set of x violating $(\mathcal{W}_{q,p})_x \overset{\zeta}{=} \mathbb{Z}$. As a $\xi\otimes\zeta$-complete component of $\mathcal{W}_{q,p}$ by Condition **(i)** in Theorem 2.3, we have $\mathcal{S} \overset{\xi\otimes\zeta}{=} (\mathcal{S}^{\mathbb{X}}\times\mathbb{Z}\cap\mathcal{W}_{q,p}) \cup (\mathbb{Z}\times\mathcal{S}^{\mathbb{Z}}\cap\mathcal{W}_{q,p}) \supseteq \mathcal{S}^{\mathbb{X}}\times\mathbb{Z}\cap\mathcal{W}_{q,p} \overset{\xi\otimes\zeta}{=} \mathcal{S}^{\mathbb{X}}\times\mathbb{Z}$. This means that $(\xi\otimes\zeta)(\mathcal{S}^{\mathbb{X}}\times\mathbb{Z}\setminus\mathcal{S}) = \int_{\mathcal{S}^{\mathbb{X}}} \zeta(\mathbb{Z}\setminus\mathcal{S}_x)\xi(\mathrm{d}x) = 0$ by Eq. (7), so for ξ-a.e. x on $\mathcal{S}^{\mathbb{X}}$, $\zeta(\mathbb{Z}\setminus\mathcal{S}_x) = 0$ [9, Thm. 15.2(ii)] thus $\mathcal{S}_x \overset{\zeta}{=} \mathbb{Z}$. So $\mathcal{S}^{\mathbb{Z}} \overset{\zeta}{=} \mathbb{Z}$. Moreover, we also have $\mathcal{S} \supseteq^{\xi\otimes\zeta} \mathbb{X}\times\mathcal{S}^{\mathbb{Z}}$ which $\overset{\xi\otimes\zeta}{=} \mathbb{X}\times\mathbb{Z}$, so we have $\mathcal{S} \overset{\xi\otimes\zeta}{=} \mathbb{X}\times\mathbb{Z}$. Similarly, from that $\mathcal{S}$ is a $\xi\otimes\zeta$-complete component also of $\mathcal{W}_{p,q}$, we have the same conclusion. □

C.4 Proof of Theorem 2.4

Proof. Let π and $\tilde{\pi}$ be two compatible joints of $p(x|z)$ and $q(z|x)$, and they are supported on the same complete support $\mathcal{S}$. By Conclusions **(2)** and **(3)** in the proof (Supplement C.2) of Theorem 2.3, there exist functions $u(x)$, $v(z)$ and $\tilde{u}(x)$, $\tilde{v}(z)$ such that $p(x|z)v(z)$ and $q(z|x)u(x)$ are the densities of π, and $p(x|z)\tilde{v}(z)$ and $q(z|x)\tilde{u}(x)$ of $\tilde{\pi}$, and $p(x|z)v(z) = q(z|x)u(x)$ and $p(x|z)\tilde{v}(z) = q(z|x)\tilde{u}(x)$, $\xi\otimes\zeta$-a.e. By the definition of a support in Lemma B.7, we know that the densities of π and $\tilde{\pi}$ are positive $\xi\otimes\zeta$-a.e. on $\mathcal{S}$, and $\int_{\mathcal{S}^{\mathbb{X}}} u \,\mathrm{d}\xi = \int_{\mathcal{S}^{\mathbb{X}}} \tilde{u} \,\mathrm{d}\xi = \int_{\mathcal{S}^{\mathbb{Z}}} v \,\mathrm{d}\zeta = \int_{\mathcal{S}^{\mathbb{Z}}} \tilde{v} \,\mathrm{d}\zeta = 1$.

Consequently, we have $\frac{p(x|z)}{q(z|x)} = \frac{u(x)}{v(z)} = \frac{\tilde{u}(x)}{\tilde{v}(z)}$, $\xi\otimes\zeta$-a.e. on $\mathcal{S}$. By Lemma B.10, for ζ-a.e. z on $\mathcal{S}^{\mathbb{Z}}$, we have $\frac{u(x)}{v(z)} = \frac{\tilde{u}(x)}{\tilde{v}(z)}$ for ξ-a.e. x on $\mathcal{S}_z$, which means that $\int_{\mathcal{S}_z} \frac{u(x)}{v(z)}\xi(\mathrm{d}x) = \int_{\mathcal{S}_z} \frac{\tilde{u}(x)}{\tilde{v}(z)}\xi(\mathrm{d}x)$. Since for ζ-a.e. z on $\mathcal{S}^{\mathbb{Z}}$, $\mathcal{S}_z \overset{\xi}{=} \mathcal{S}^{\mathbb{X}}$, we have by Lemma B.3 that $\int_{\mathcal{S}^{\mathbb{X}}} \frac{u(x)}{v(z)}\xi(\mathrm{d}x) = \int_{\mathcal{S}^{\mathbb{X}}} \frac{\tilde{u}(x)}{\tilde{v}(z)}\xi(\mathrm{d}x)$, which in turn gives $\frac{1}{v(z)} \int_{\mathcal{S}^{\mathbb{X}}} u \,\mathrm{d}\xi = \frac{1}{v(z)} = \frac{1}{\tilde{v}(z)} \int_{\mathcal{S}^{\mathbb{X}}} \tilde{u} \,\mathrm{d}\xi = \frac{1}{\tilde{v}(z)}$. So $v(z) = \tilde{v}(z)$ for ζ-a.e. z on $\mathcal{S}^{\mathbb{Z}}$, and similarly $u(x) = \tilde{u}(x)$ for ξ-a.e. x on $\mathcal{S}^{\mathbb{X}}$. Subsequently, the density $p(x|z)v(z)$ or $q(z|x)u(x)$ of π is $\xi\otimes\zeta$-a.e. the same as the density $p(x|z)\tilde{v}(z)$ or $q(z|x)\tilde{u}(x)$ of $\tilde{\pi}$. Hence, π and $\tilde{\pi}$ are the same distribution. □

C.5 The Dirac Compatibility Lemma

Before proving the main instructive compatibility theorem (2.6) for the Dirac case, we first present an existential equivalent criterion for compatibility, which provides insights to the problem.

Lemma C.5 (Dirac compatibility, existential)**.** *Conditional distribution $\nu(\mathcal{Z}|x)$ is compatible with $\mu(\mathcal{X}|z) := \delta_{f(z)}(\mathcal{X})$ where function $f : \mathbb{Z} \to \mathbb{X}$ is $\mathscr{X}/\mathscr{Z}$-measurable, if and only if there is a distribution β on $(\mathbb{Z}, \mathscr{Z})$ such that $\nu(\mathcal{Z}|x) = \frac{\mathrm{d}\beta(\mathcal{Z}\cap f^{-1}(\cdot))}{\mathrm{d}\beta(f^{-1}(\cdot))}(x)$, and this β is the marginal $\pi^{\mathbb{Z}}$ of a compatible joint π of them.*

Proof. We first show the validity of the R-N derivative. Since β is a distribution thus a finite measure, $\beta(\mathcal{Z}\cap f^{-1}(\cdot))$ and $\beta(f^{-1}(\cdot))$ are also finite thus sigma-finite. For any $\mathcal{X} \in \mathscr{X}$ such that $\beta(f^{-1}(\mathcal{X})) = 0$, we have $\beta(\mathcal{Z}\cap f^{-1}(\mathcal{X})) \leqslant \beta(f^{-1}(\mathcal{X})) = 0$ since $\mathcal{Z}\cap f^{-1}(\mathcal{X}) \subseteq f^{-1}(\mathcal{X})$ and measures are monotone. So $\beta(\mathcal{Z}\cap f^{-1}(\mathcal{X})) = 0$ and $\beta(\mathcal{Z}\cap f^{-1}(\cdot)) \ll \beta(f^{-1}(\cdot))$. By the R-N theorem [9, Thm. 32.2], the R-N derivative exists.

"Only if" (necessity): Let π be a compatible joint. Since μ and ν are its conditional distributions, by Eq. (11), we have:

$$\pi(\mathcal{X}\times\mathcal{Z}) = \int_{\mathcal{Z}} \mu(\mathcal{X}|z)\pi^{\mathbb{Z}}(\mathrm{d}z) = \int_{\mathcal{X}} \nu(\mathcal{Z}|x)\pi^{\mathbb{X}}(\mathrm{d}x), \quad \forall \mathcal{X}\times\mathcal{Z} \in \mathscr{X}\times\mathscr{Z}.$$

The first integral is $\int_{\mathcal{Z}} \mathbb{I}[f(z) \in \mathcal{X}]\pi^{\mathbb{Z}}(\mathrm{d}z) = \int_{\mathcal{Z}} \mathbb{I}[z \in f^{-1}(\mathcal{X})]\pi^{\mathbb{Z}}(\mathrm{d}z) = \pi^{\mathbb{Z}}(\mathcal{Z}\cap f^{-1}(\mathcal{X}))$. Particularly, $\pi^{\mathbb{X}}(\mathcal{X}) = \pi(\mathcal{X}\times\mathbb{Z}) = \pi^{\mathbb{Z}}(f^{-1}(\mathcal{X}))$, *i.e.* $\pi^{\mathbb{X}}$ is the transformed (pushed-forward) distribution from $\pi^{\mathbb{Z}}$ by measurable function f [9, p.196]. On the other hand, the equality to the second integral means that $\pi^{\mathbb{Z}}(\mathcal{Z}\cap f^{-1}(\mathcal{X})) = \int_{\mathcal{X}} \nu(\mathcal{Z}|x)\pi^{\mathbb{X}}(\mathrm{d}x) = \int_{\mathcal{X}} \nu(\mathcal{Z}|x)\pi^{\mathbb{Z}}(f^{-1}(\mathrm{d}x))$. This means that $\nu(\mathcal{Z}|x)$ is the R-N derivative of $\mathcal{X} \mapsto \pi^{\mathbb{Z}}(\mathcal{Z}\cap f^{-1}(\mathcal{X}))$ w.r.t $\mathcal{X} \mapsto \pi^{\mathbb{Z}}(f^{-1}(\mathcal{X}))$. Taking β as $\pi^{\mathbb{Z}}$, which is a distribution on $(\mathbb{Z}, \mathscr{Z})$, yields the necessary condition.

"If" (sufficiency): For any measurable rectangle $\mathcal{X}\times\mathcal{Z} \in \mathscr{X}\times\mathscr{Z}$, define $\pi(\mathcal{X}\times\mathcal{Z}) := \int_{\mathcal{Z}} \mu(\mathcal{X}|z)\beta(\mathrm{d}z)$ and $\tilde{\pi}(\mathcal{X}\times\mathcal{Z}) := \beta(\mathcal{Z}\cap f^{-1}(\mathcal{X}))$. Since for any $z \in \mathbb{Z}$, $f(z) \in \mathbb{X}$, so $\pi(\mathbb{X}\times\mathbb{Z}) = \int_{\mathbb{Z}} \mu(\mathbb{X}|z)\beta(\mathrm{d}z) = \int_{\mathbb{Z}} \beta(\mathrm{d}z) = 1$. Since $f^{-1}(\mathbb{X}) = \mathbb{Z}$, we have $\tilde{\pi}(\mathbb{X}\times\mathbb{Z}) = \beta(\mathbb{Z}) = 1$. So both π and $\tilde{\pi}$ are finite thus sigma-finite. Moreover, for any $\mathcal{X}\times\mathcal{Z} \in \mathscr{X}\times\mathscr{Z}$, we have $\pi(\mathcal{X}\times\mathcal{Z}) = \int_{\mathcal{Z}} \mathbb{I}[f(z) \in \mathcal{X}]\beta(\mathrm{d}z) = \int_{\mathcal{Z}} \mathbb{I}[z \in f^{-1}(\mathcal{X})]\beta(\mathrm{d}z) = \int_{\mathcal{Z}\cap f^{-1}(\mathcal{X})} \beta(\mathrm{d}z) = \beta(\mathcal{Z}\cap f^{-1}(\mathcal{X})) = \tilde{\pi}(\mathcal{X}\times\mathcal{Z})$, *i.e.* π and $\tilde{\pi}$ agree on the pi-system $\mathscr{X}\times\mathscr{Z}$. So by Billingsley [9, Thm. 10.3], π and $\tilde{\pi}$ extend to the same distribution (probability measure) on $(\mathbb{X}\times\mathbb{Z}, \mathscr{X}\otimes\mathscr{Z})$.

On the other hand, we have $\pi^{\mathbb{Z}}(\mathcal{Z}) = \pi(\mathbb{X}\times\mathcal{Z}) = \int_{\mathcal{Z}} \mu(\mathbb{X}|z)\beta(\mathrm{d}z) = \int_{\mathcal{Z}} \beta(\mathrm{d}z) = \beta(\mathcal{Z})$, and furthermore from this, μ is a conditional distribution of π due to its construction and Eq. (11). Moreover, $\tilde{\pi}^{\mathbb{X}}(\mathcal{X}) = \tilde{\pi}(\mathcal{X}\times\mathbb{Z}) = \beta(\mathbb{Z}\cap f^{-1}(\mathcal{X})) = \beta(f^{-1}(\mathcal{X}))$, and by the definition of $\nu(\mathcal{Z}|x)$ as an R-N derivative, we have $\beta(\mathcal{Z}\cap f^{-1}(\mathcal{X})) = \int_{\mathcal{X}} \nu(\mathcal{Z}|x)\beta(f^{-1}(\mathrm{d}x))$, which is $\tilde{\pi}(\mathcal{X}\times\mathcal{Z}) = \int_{\mathcal{X}} \nu(\mathcal{Z}|x)\tilde{\pi}^{\mathbb{X}}(\mathrm{d}x)$. So again due to Eq. (11), ν is a conditional distribution of $\tilde{\pi}$. Since π and $\tilde{\pi}$ are the same distribution on $(\mathbb{X}\times\mathbb{Z}, \mathscr{X}\otimes\mathscr{Z})$, we know that μ and ν are compatible. □

Key insights. Let π be a compatible joint of $\mu(\mathcal{X}|z) := \delta_{f(z)}(\mathcal{X})$ and $\nu(\mathcal{Z}|x)$. For any $\mathcal{X}\times\mathcal{Z} \in \mathscr{X}\times\mathscr{Z}$, we have:

$$\pi(\mathcal{X}\times\mathcal{Z}) = \pi^{\mathbb{Z}}(\mathcal{Z}\cap f^{-1}(\mathcal{X})) = \int_{\mathcal{X}} \nu(\mathcal{Z}|x)\pi^{\mathbb{Z}}(f^{-1}(\mathrm{d}x)) = \int_{f^{-1}(\mathcal{X})} \nu(\mathcal{Z}|f(z))\pi^{\mathbb{Z}}(\mathrm{d}z),$$

where the last equality holds due to the rule of change of variables [9, Thm. 16.13]. Let $f^{-1}(\mathscr{X}) := \sigma(\{f^{-1}(\mathcal{X}) \mid \mathcal{X} \in \mathscr{X}\})$ be the pulled-back sigma-field from $\mathscr{X}$ by f. It is a sub-sigma-field of $\mathscr{Z}$ as every $f^{-1}(\mathcal{X}) \in \mathscr{Z}$ since f is measurable. So the last equality means that:

$$\nu(\mathcal{Z}|f(z)) = \frac{\mathrm{d}\pi^{\mathbb{Z}}(\mathcal{Z} \cap \cdot)}{\mathrm{d}\pi^{\mathbb{Z}}(\cdot)}\bigg|_{f^{-1}(\mathscr{X})}(z).$$

The expression on the left makes sense since for all values of z that yield the same value of $f(z)$, the R-N derivative is the same. The second equality also gives:

$$\nu(\mathcal{Z}|x) = \frac{\mathrm{d}\pi^{\mathbb{Z}}(\mathcal{Z} \cap f^{-1}(\cdot))}{\mathrm{d}\pi^{\mathbb{Z}}(f^{-1}(\cdot))}\bigg|_{\mathscr{X}}(x).$$

C.6 Proof of Theorem 2.6

Proof. **"Only if" (necessity):** Suppose that $\nu(\mathcal{Z}|x)$ and $\mu(\mathcal{X}|z) := \delta_{f(z)}(\mathcal{X})$ are compatible but for *any* $x \in \mathbb{X}$, $\nu(f^{-1}(\{x\})|x) < 1$. Consider the set $\mathcal{S} := \{(f(z), z) \mid z \in \mathbb{Z}\}$. Since f is $\mathscr{X}/\mathscr{Z}$-measurable, this set $\mathcal{S}$ is $\mathscr{X} \otimes \mathscr{Z}$-measurable. It is also easy to verify that $\mathcal{S}_z = \{f(z)\}$ and $\mathcal{S}_x = f^{-1}(\{x\})$. Now let π be *any* of their compatible joint distribution. From Eq. (12), we know that $\pi(\mathcal{S}) = \int_{\mathbb{Z}} \mu(\mathcal{S}_z|z)\pi^{\mathbb{Z}}(\mathrm{d}z) = \int_{\mathbb{Z}} \delta_{f(z)}(\{f(z)\})\pi^{\mathbb{Z}}(\mathrm{d}z) = \int_{\mathbb{Z}} \pi^{\mathbb{Z}}(\mathrm{d}z) = \pi^{\mathbb{Z}}(\mathbb{Z}) = 1$. On the other hand, also from Eq. (12) and due to the compatibility, we have $\pi(\mathcal{S}) = \int_{\mathbb{X}} \nu(\mathcal{S}_x|x)\pi^{\mathbb{X}}(\mathrm{d}x) = \int_{\mathbb{X}} \nu(f^{-1}(\{x\})|x)\pi^{\mathbb{X}}(\mathrm{d}x) < \int_{\mathbb{X}} \pi^{\mathbb{X}}(\mathrm{d}x) = \pi^{\mathbb{X}}(\mathbb{X}) = 1$, which leads to a contradiction. So if $\nu(\mathcal{Z}|x)$ and $\mu(\mathcal{X}|z)$ are compatible, then there is $x_0 \in \mathbb{X}$ such that $\nu(f^{-1}(\{x_0\})|x_0) = 1$.

"If" (sufficiency): Let $\beta(\mathcal{Z}) := \nu(f^{-1}(\{x_0\}) \cap \mathcal{Z}|x_0)$ be a set function on $\mathscr{Z}$. We can verify that this β is a distribution (probability measure) on $(\mathbb{Z}, \mathscr{Z})$ since $\nu(\cdot|x_0)$ is. Particularly, since f is $\mathscr{X}/\mathscr{Z}$-measurable and $\{x_0\} \in \mathscr{X}$ due to the assumption, we know that $f^{-1}(\{x_0\})$ thus $f^{-1}(\{x_0\}) \cap \mathcal{Z}$ for any $\mathcal{Z} \in \mathscr{Z}$ are in $\mathscr{Z}$; $\beta(\emptyset) = \nu(\emptyset|x_0) = 0$; $\beta(\mathbb{Z}) = \nu(f^{-1}(\{x_0\})|x_0) = 1$ according to the assumption; for any countable disjoint $\mathscr{Z}$-sets $\mathcal{Z}^{(1)}, \mathcal{Z}^{(2)}, \cdots$, it holds that $\mathcal{Z}^{(1)} \cap f^{-1}(\{x_0\}), \mathcal{Z}^{(2)} \cap f^{-1}(\{x_0\}), \cdots$ are also disjoint $\mathscr{Z}$-sets, so $\beta(\bigcup_{i=1}^{\infty} \mathcal{Z}^{(i)}) = \nu(f^{-1}(\{x_0\}) \cap \bigcup_{i=1}^{\infty} \mathcal{Z}^{(i)}|x_0) = \nu(\bigcup_{i=1}^{\infty} f^{-1}(\{x_0\}) \cap \mathcal{Z}^{(i)}|x_0) = \sum_{i=1}^{\infty} \nu(f^{-1}(\{x_0\}) \cap \mathcal{Z}^{(i)}|x_0) = \sum_{i=1}^{\infty} \beta(\mathcal{Z}^{(i)})$.

Now we prove that $\beta(\mathcal{Z} \cap f^{-1}(\mathcal{X})) = \int_{\mathcal{X}} \nu(\mathcal{Z}|x)\beta(f^{-1}(\mathrm{d}x)), \forall \mathcal{X} \times \mathcal{Z} \in \mathscr{X} \times \mathscr{Z}$ which is sufficient due to Lemma C.5. For any $\mathcal{X} \times \mathcal{Z} \in \mathscr{X} \times \mathscr{Z}$, the l.h.s is $\beta(\mathcal{Z} \cap f^{-1}(\mathcal{X})) = \nu(f^{-1}(\{x_0\}) \cap f^{-1}(\mathcal{X}) \cap \mathcal{Z}|x_0) = \nu(f^{-1}(\{x_0\}) \cap \mathcal{Z}|x_0)\mathbb{I}[x_0 \in \mathcal{X}]$, where the last equality holds since $z \in f^{-1}(\{x_0\}) \cap f^{-1}(\mathcal{X})$ if and only if $f(z) = x_0 \in \mathcal{X}$. The integral on the r.h.s is $\int_{\mathcal{X}} \nu(\mathcal{Z}|x)\nu(f^{-1}(\{x_0\}) \cap f^{-1}(\mathrm{d}x)|x_0)$. Since the measure $\mathcal{X} \mapsto \nu(f^{-1}(\{x_0\}) \cap f^{-1}(\mathcal{X})|x_0)$ is zero on the set $\mathcal{X} \setminus \{x_0\}$ (if there is any $z \in f^{-1}(\{x_0\}) \cap f^{-1}(\mathcal{X} \setminus \{x_0\})$, then we have $f(z) = x_0$ and $f(z) \in \mathcal{X} \setminus \{x_0\}$, which is a contradiction), the integral can be reduced on $\{x_0\} \cap \mathcal{X}$ [9, Thm. 16.9]: $\int_{\{x_0\} \cap \mathcal{X}} \nu(\mathcal{Z}|x)\nu(f^{-1}(\{x_0\}) \cap f^{-1}(\mathrm{d}x)|x_0) = \mathbb{I}[x_0 \in \mathcal{X}]\nu(\mathcal{Z}|x_0)\nu(f^{-1}(\{x_0\})|x_0) = \nu(\mathcal{Z}|x_0)\mathbb{I}[x_0 \in \mathcal{X}]$. Moreover, $\nu(\mathcal{Z}|x_0) = \nu(\mathcal{Z} \cap f^{-1}(\{x_0\})|x_0) + \nu(\mathcal{Z} \setminus f^{-1}(\{x_0\})|x_0)$ where $\nu(\mathcal{Z} \setminus f^{-1}(\{x_0\})|x_0) \leqslant \nu(\mathbb{Z} \setminus f^{-1}(\{x_0\})|x_0) = 1 - \nu(f^{-1}(\{x_0\})|x_0) = 0$, we have $\nu(\mathcal{Z} \setminus f^{-1}(\{x_0\})|x_0) = 0$ and $\nu(\mathcal{Z}|x_0) = \nu(\mathcal{Z} \cap f^{-1}(\{x_0\})|x_0)$. So the integral on the r.h.s is $\nu(\mathcal{Z} \cap f^{-1}(\{x_0\})|x_0)\mathbb{I}[x_0 \in \mathcal{X}]$, which is the same as the l.h.s. So the equality is verified. $\square$

D Topics on the Methods of CyGen

D.1 Relation to other auto-encoder regularizations

There are methods that consider regularizing the standard auto-encoder (AE) [54, 4] with deterministic encoder $g(x)$ and decoder $f(z)$ for certain robustness. These regularizations are introduced in addition to the standard AE loss, *i.e.* the reconstruction loss: $\mathbb{E}_{p^*(x)}\ell(x, f(g(x)))$, where $\ell(x, x')$ is a measure of similarity between x and x'. If $\ell(x, f(z))$ can be treated as a (scaled) negative log-likelihood $-\log p(x|z)$ on $\mathbb{X}$ (*e.g.*, squared 2-norm ℓ for a Gaussian $p(x|z)$, cross entropy ℓ for a Bernoulli/categorical $p(x|z)$), then we can adopt a distributional view of the decoder as $p(x|z)$ and the encoder as $\delta_{g(x)}(z)$ [11], and reformulate the reconstruction loss also under the distributional view: $\mathbb{E}_{p^*(x)}[-\log p(x|g(x))] = \mathbb{E}_{p^*(x)\delta_{g(x)}(z)}[-\log p(x|z)]$.

[11]This is the notation of a Dirac's delta function, which is not a function in the usual sense. We adopt this form for the similarity to the DAE loss.

Comparison with Jacobian norm regularizations. Contractive AE (CAE) [51, 52] regularizes the Jacobian norm of the encoder, $\lambda \mathbb{E}_{p^*(x)} \big\| \nabla_x g^\top(x) \big\|_F^2$ (λ controls the scale), in hope to encourage the robustness of the encoded representation against local changes around training data. When it is combined with the reconstruction loss which preserves data variation in the representation for reconstruction, the robustness is confined to the orthogonal direction to the data manifold, which often does not reflect semantic meanings of interest. In other words, the variation in this orthogonal direction is contracted in the representation, hence the name. When applied to a linear encoder, this becomes the well-known weight-decay regularizer.

Denoising AE (DAE) [61, 6, 7] considers the robustness to random corruption/perturbation on data, so its encoding process is $z = g(x + \epsilon_e)$ where $\epsilon_e \sim \mathcal{N}(0, \sigma_e^2 I_{d_\mathbb{X}})$ (or any other distribution with $\mathbb{E}[\epsilon_e] = 0$ and $\mathrm{Var}[\epsilon_e] = \sigma_e^2 I_{d_\mathbb{X}}$), which defines a probabilistic encoder $q(z|x)$ (note that this is different from an additive Gaussian encoder). The goal for training a DAE is thus to try to reconstruct the input under the random corruption, by minimizing the DAE loss: $\mathbb{E}_{p^*(x)q(z|x)}[-\log p(x|z)]$, which resembles the distributional form of the standard reconstruction loss. For infinitesimal corruption variance σ_e^2 and squared 2-norm ℓ, the DAE loss is roughly equivalent to regularizing the standard reconstruction loss with $\sigma_e^2 \mathbb{E}_{p^*(x)} \big\| \nabla_x (f \circ g)^\top(x) \big\|_F^2$, *i.e.* the Jacobian norm of the reconstruction function [51, 1]. So DAE can be viewed to promote the robustness of reconstruction while CAE of the representation [51].

In contrast, for additive Gaussian decoder (*i.e.*, squared 2-norm ℓ) and encoder, our compatibility regularization Eq. (2) is $\mathbb{E}_{\rho(x,z)} \Big\| \frac{1}{\sigma_d^2} \big(\nabla_z f^\top(z) \big)^\top - \frac{1}{\sigma_e^2} \nabla_x g^\top(x) \Big\|_F^2$, which is different from CAE and DAE regularizations. Ideologically, the compatibility loss is an intrinsic constraint to make use of the distributional nature of the encoder and decoder, and is not motivated from the additional requirement of robustness in some sense.

Comparison with a more accurate DAE reformulation. In fact, the analysis in [51, 1] for DAE as a regularization of the reconstruction loss is inaccurate. Key ingredients for the analysis are the Taylor expansions: $\|x + \varepsilon\|_2^2 = \|x\|_2^2 + 2x^\top \varepsilon + \varepsilon^\top \varepsilon$, $\exp\{x + \varepsilon\} = \exp\{x\}(1 + \varepsilon + \frac{1}{2}\varepsilon^2) + o(\varepsilon^2)$, and $\log(1 + \varepsilon) = \varepsilon - \frac{1}{2}\varepsilon^2 + o(\varepsilon^2)$. In the following, we consider $\ell(x, x') = \|x - x'\|_2^2$, corresponding to an additive Gaussian decoder $p(x|z)$.

First consider the additive Gaussian encoder, $q(z|x) = \mathcal{N}(z|g(x), \sigma_e^2 I_{d_\mathbb{Z}})$, or $z = g(x) + \epsilon_e, \epsilon_e \sim \mathcal{N}(0, \sigma_e^2 I_{d_\mathbb{Z}})$. Consider the case for infinitesimal σ_e. For the DAE loss, we have (omitting the expectation over $p^*(x)$):

$$
\begin{aligned}
&\mathbb{E}_{q(z|x)}[-\log p(x|z)] = \mathbb{E}_{q(z|x)}[\ell(x, f(z))] = \mathbb{E}_{q(z|x)} \|x - f(z)\|_2^2 = \mathbb{E}_{p(\epsilon_e)} \|x - f(g(x) + \epsilon_e)\|_2^2 \\
= {}& \mathbb{E}_{p(\epsilon_e)} \left[\left\| x - f(g(x)) - (\nabla f^\top)^\top \epsilon_e - \frac{1}{2} \epsilon_e^\top (\nabla^2 f) \epsilon_e + o(\epsilon_e^2) \right\|_2^2 \right] \\
= {}& \mathbb{E}_{p(\epsilon_e)} \Big[\|x - f(g(x))\|_2^2 - 2\big(x - f(g(x))\big)^\top \Big((\nabla f^\top)^\top \epsilon_e + \frac{1}{2} \epsilon_e^\top (\nabla^2 f) \epsilon_e \Big) \\
&\quad + \epsilon_e^\top (\nabla f^\top)(\nabla f^\top)^\top \epsilon_e + o(\epsilon_e^2) \Big] \\
= {}& \ell\big(x, f(g(x))\big) - \sigma_e^2 \big(x - f(g(x))\big)^\top \Delta f + \sigma_e^2 \big\| \nabla f^\top \big\|_F^2 + o(\sigma_e^2),
\end{aligned} \tag{19}
$$

where $(\nabla f^\top)^\top$ is the Jacobian of f, $(\epsilon_e^\top (\nabla^2 f) \epsilon_e)_i := \sum_{j,k=1..d_\mathbb{Z}} (\epsilon_e)_i (\epsilon_e)_j \partial_{z_i} \partial_{z_j} f_i$, and $(\Delta f)_i := \sum_{j=1..d_\mathbb{Z}} \partial_{z_j} \partial_{z_j} f_i$, and they are evaluated at $z = g(x)$. Note that in addition to the Jacobian norm regularization term discovered in [51, 1], there is a second regularization term $-\sigma_e^2 \big(x - f(g(x))\big)^\top \Delta f$ that DAE imposes.

For the data-fitting loss of CyGen Eq. (4), a similar approximation can be derived (again, omitting the expectation over $p^*(x)$):

$$
\begin{aligned}
&\log \mathbb{E}_{q(z|x)}[1/p(x|z)] = \log \mathbb{E}_{q(z|x)} \exp\{-\log p(x|z)\} = \log \mathbb{E}_{q(z|x)} \exp\{\ell(x, f(z))\} \\
= {}& \log \mathbb{E}_{q(z|x)} \exp\{\|x - f(z)\|_2^2\} = \log \mathbb{E}_{p(\epsilon_e)} \exp\{\|x - f(g(x) + \epsilon_e)\|_2^2\} \\
= {}& \log \mathbb{E}_{p(\epsilon_e)} \exp\left\{ \left\| x - f(g(x)) - (\nabla f^\top)^\top \epsilon_e - \frac{1}{2} \epsilon_e^\top (\nabla^2 f) \epsilon_e + o(\epsilon_e^2) \right\|_2^2 \right\}
\end{aligned}
$$

$$
\begin{aligned}
&= \log \mathbb{E}_{p(\epsilon_e)} \exp\Big\{ \|x - f(g(x))\|_2^2 - 2\big(x - f(g(x))\big)^\top \Big((\nabla f^\top)^\top \epsilon_e + \frac{1}{2} \epsilon_e^\top (\nabla^2 f) \epsilon_e \Big) \\
&\quad + \epsilon_e^\top (\nabla f^\top)(\nabla f^\top)^\top \epsilon_e + o(\epsilon_e^2) \Big\} \\
&= \log \mathbb{E}_{p(\epsilon_e)} \Big[\exp\{\|x - f(g(x))\|_2^2\} \Big(1 - 2\big(x - f(g(x))\big)^\top \Big((\nabla f^\top)^\top \epsilon_e + \frac{1}{2} \epsilon_e^\top (\nabla^2 f) \epsilon_e \Big) \\
&\quad + \epsilon_e^\top (\nabla f^\top)(\nabla f^\top)^\top \epsilon_e + 2\Big(\big(x - f(g(x))\big)^\top (\nabla f^\top)^\top \epsilon_e \Big)^2 + o(\epsilon_e^2) \Big) \Big] \\
&= \log \Big[\exp\{\|x - f(g(x))\|_2^2\} \Big(1 - \sigma_e^2 \big(x - f(g(x))\big)^\top \Delta f \\
&\quad + \sigma_e^2 \big\| \nabla f^\top \big\|_F^2 + 2\sigma_e^2 \big\| (\nabla f^\top)\big(x - f(g(x))\big) \big\|_2^2 + o(\sigma_e^2) \Big) \Big] \\
&= \ell\big(x - f(g(x))\big) - \sigma_e^2 \big(x - f(g(x))\big)^\top \Delta f + \sigma_e^2 \big\| \nabla f^\top \big\|_F^2 + 2\sigma_e^2 \big\| (\nabla f^\top)\big(x - f(g(x))\big) \big\|_2^2 + o(\sigma_e^2).
\end{aligned}
$$

This is different from the regularization interpretation of DAE Eq. (19) as a third regularization term $2\sigma_e^2 \big\| (\nabla f^\top)\big(x - f(g(x))\big) \big\|_2^2$ is presented.

The compatibility loss Eq. (2) in CyGen becomes: $\mathbb{E}_{\rho(x,z)} \Big\| \frac{1}{\sigma_d^2} \big(\nabla_z f^\top(z) \big)^\top - \frac{1}{\sigma_e^2} \nabla_x g^\top(x) \Big\|_F^2$, where σ_d^2 is the Gaussian variance of the decoder $p(x|z)$ (inverse scale for $\ell(\cdot,\cdot)$). When $\rho(x,z) = p^*(x) q(z|x)$, this can be further reduced to (omitting the expectation over $p^*(x)$):

$$
\begin{aligned}
&\mathbb{E}_{q(z|x)} \Big\| \frac{1}{\sigma_d^2} \big(\nabla_z f^\top(z) \big)^\top - \frac{1}{\sigma_e^2} \nabla_x g^\top(x) \Big\|_F^2 = \mathbb{E}_{p(\epsilon_e)} \Big\| \frac{1}{\sigma_d^2} \big(\nabla f^\top(g(x) + \epsilon_e) \big)^\top - \frac{1}{\sigma_e^2} \nabla g^\top \Big\|_F^2 \\
&= \mathbb{E}_{p(\epsilon_e)} \Big\| \frac{1}{\sigma_d^2} \Big((\nabla f^\top)^\top + (\nabla^2 f^\top)^\top \epsilon_e + \frac{1}{2} \epsilon_e^\top (\nabla^3 f^\top)^\top \epsilon_e + o(\epsilon_e^2) \Big) - \frac{1}{\sigma_e^2} \nabla g^\top \Big\|_F^2 \\
&= \Big\| \frac{1}{\sigma_d^2} (\nabla f^\top)^\top - \frac{1}{\sigma_e^2} \nabla g^\top \Big\|_F^2 + \frac{\sigma_e^2}{\sigma_d^4} (\nabla f^\top) : (\nabla \Delta f^\top) + \frac{\sigma_e^2}{\sigma_d^4} \big\| \nabla^2 f^\top \big\|_F^2 + o(\sigma_e^2),
\end{aligned}
$$

where $\big((\nabla^2 f^\top)^\top \epsilon_e \big)_{ij} := \sum_{k=1..d_{\mathbb{Z}}} (\epsilon_e)_k \partial_{z_k} \partial_{z_j} f_i$, $\big(\epsilon_e^\top (\nabla^3 f^\top)^\top \epsilon_e \big)_{ij} := \sum_{k,k'=1..d_{\mathbb{Z}}} (\epsilon_e)_k (\epsilon_e)_{k'} \partial_{z_k} \partial_{z_{k'}} \partial_{z_j} f_i$, and $(\nabla f^\top) : (\nabla \Delta f^\top) := \sum_{\substack{i=1..d_{\mathbb{X}},\\ j,k=1..d_{\mathbb{Z}}}} (\partial_{z_j} f_i)(\partial_{z_j} \partial_{z_k} \partial_{z_k} f_i)$, $\big\| \nabla^2 f^\top \big\|_F^2 := \sum_{\substack{i=1..d_{\mathbb{X}},\\ j,k=1..d_{\mathbb{Z}}}} \big(\partial_{z_k} \partial_{z_j} f_i \big)^2$, and all terms are evaluated at $z = g(x)$. This is different from the regularization of CAE and the regularization explanation of DAE.

For the corruption encoder, $z = g(x + \epsilon_e), \epsilon_e \sim \mathcal{N}(0, \sigma_e^2 I_{d_{\mathbb{X}}})$, approximations of the DAE loss and the data-fitting loss of CyGen are similar to the above expansions except that derivatives of f are replaced with those of $f \circ g$. Particularly, from Eq. (19), we find that the conclusion in [51, 1] missed the term $-\sigma_e^2 \big(x - f(g(x))\big)^\top \Delta(f \circ g)$ that is also of order σ_e^2. For the compatibility loss, as there is no explicit expression of $\log q(z|x)$ (unless $g(x)$ is invertible), the above expression does not hold. But anyway, it is different from CAE and DAE regularizations.

Relation to the tied weights trick. The compatibility loss also explains the "tied weights" trick in AE, which is widely adopted and vital for the success of AE [61, 51, 1]. The trick is considered when components of x and z are binary, and a one-layer, product-of-Bernoulli encoder $q(z|x) = \prod_{j=1}^{d_{\mathbb{Z}}} \mathrm{Bern}(z_j | s((W_e)_{j,:} x + (b_e)_j))$ and decoder $p(x|z) = \prod_{i=1}^{d_{\mathbb{X}}} \mathrm{Bern}(x_i | s((W_d)_{i,:} z + (b_d)_i))$ are used, where $s(l) := 1/(1 + \exp\{-l\})$ denotes the sigmoid activation function. For the encoder, we have $q(z|x) = \frac{\exp\{z^\top (W_e x + b_e)\}}{\prod_{j=1}^{d_{\mathbb{Z}}} (1 + \exp\{(W_e)_{j,:} x + (b_e)_j\})}$ thus $\log q(z|x) = z^\top (W_e x + b_e) - \sum_{j=1}^{d_{\mathbb{Z}}} \log(1 + \exp\{(W_e)_{j,:} x + (b_e)_j\})$, so $\nabla_x \nabla_z^\top \log q(z|x) = W_e^\top$. Similarly for the decoder, we have $\nabla_x \nabla_z^\top \log p(x|z) = W_d$. So the compatibility loss Eq. (2) in this case is $\big\| W_d - W_e^\top \big\|_F^2$, which leads to $W_d = W_e^\top$ when it is zero. This recovers the tied weight trick.

In this Bernoulli case, the CAE regularizer is $\mathbb{E}_{p^*(x)} \sum_{j=1}^{d_{\mathbb{Z}}} \frac{\exp\{-2((W_e)_{j,:} x + (b_e)_j)\} \sum_{i=1}^{d_{\mathbb{X}}} (W_e)_{ji}^2}{\big(1 + \exp\{-((W_e)_{j,:} x + (b_e)_j)\}\big)^4} = \mathbb{E}_{p^*(x)} \sum_{j=1}^{d_{\mathbb{Z}}} s((W_e)_{j,:} x + (b_e)_j)^2 \big(1 - s((W_e)_{j,:} x + (b_e)_j)\big)^2 \sum_{i=1}^{d_{\mathbb{X}}} (W_e)_{ji}^2$ and DAE does not have the Jacobian-norm regularization explanation, so they are different from the compatibility loss.

D.2 Gradient estimation for flow-based models without tractable inverse

Flow-based density models. As the insight we draw from the analysis on Gaussian VAE in Sec. 3.1, it is inappropriate to implement both conditionals $p_\theta(x|z)$, $q_\phi(z|x)$ using additive Gaussian models. So we need more flexible and expressive probabilistic models that also allow explicit density evaluation (so implicit models like GANs are not suitable). Flow-based models [16, 44, 32, 5, 12] are a good choice. They also allow direct sampling with reparameterization for efficiently estimating and optimizing the data-fitting loss Eq. (4) (for which energy-based models are costly), and have been used as the inference model $q_\phi(z|x)$ of VAEs [49, 34, 59, 22]. For a connection to these prior works, we use a flow-based model also for the inference model $q_\phi(z|x)$. An additive-Gaussian likelihood model $p_\theta(x|z)$ is then allowed for learning nonlinear representations.

To define the distribution $q_\phi(z|x)$, a flow-based model uses a parameterized *invertible* differentiable transformation $z = T_\phi(e|x)$ to map a random seed e (of the same dimension $d_\mathbb{Z}$) following a simple base distribution $p(e)$ [12](*e.g.*, a standard Gaussian) to $\mathbb{Z} = \mathbb{R}^{d_\mathbb{Z}}$. By deliberately designed architectures, the transformation $T_\phi(\cdot|x)$ is guaranteed to be invertible, yet still being expressive, with some examples that are even universal approximators [58]. Benefited from the invertibility, the defined density can be explicitly given by the rule of change of variables [9, Thm. 17.2]:

$$q_\phi(z|x) = p(e = T_\phi^{-1}(z|x))\left|\nabla_z T_\phi^{-\top}(z|x)\right|,$$

where $\left|\nabla_z T_\phi^{-\top}(z|x)\right|$ is the absolute value of the determinant of the Jacobian of $T_\phi^{-1}(z|x)$ (w.r.t z).

Problem for evaluating the compatibility loss. Although $T_\phi(z|x)$ is guaranteed to be invertible, in common instances computing its inverse is intractable [49, 34, 59] or costly [22, 5, 12] (however, they all guarantee an easy calculation of the Jacobian determinant $\left|\nabla_z T_\phi^{-\top}(z|x)\right|$ for efficient density evaluation). This means that density estimation of $q_\phi(z|x)$ is intractable for an arbitrary z value, but is only possible for a generated z value, whose inverse e is known in advance (the generated z is computed from this e). This however, introduces problems when computing the gradients $\nabla_x \log q_\phi(z|x)$, $\nabla_z \log q_\phi(z|x)$ for the compatibility loss (Eq. (2) or Eq. (3)).

To see this, it is important to distinguish the "formal arguments" and "actual arguments" of a function. It makes a difference when taking derivatives if the actual arguments are fed to formal arguments in an involved way. What we need is the derivatives w.r.t the formal arguments, but automatic differentiation tools (*e.g.*, the `autograd` utility in PyTorch [45]) could only compute the derivatives w.r.t the actual arguments. We use capital subscripts for formal arguments and lowercase letters for actual arguments. Following this rule, we denote $\log q^\phi_{Z|X}(z|x)$ for $\log q_\phi(z|x)$ above, so $\nabla_Z \log q^\phi_{Z|X}$ denotes the gradient function that differentiates the first formal argument Z of $\log q^\phi_{Z|X}$, and similarly for $\nabla_X \log q^\phi_{Z|X}$. Then at a generated value of $z = T_\phi(e|x)$ from a random seed e, the required gradients in the compatibility loss are w.r.t to the formal arguments $\nabla_Z \log q^\phi_{Z|X}(T_\phi(e|x)|x)$ and $\nabla_X \log q^\phi_{Z|X}(T_\phi(e|x)|x)$, while automatic differentiation tools could only give the gradients w.r.t the actual arguments $\nabla_e \log q^\phi_{Z|X}(T_\phi(e|x)|x)$ and $\nabla_x \log q^\phi_{Z|X}(T_\phi(e|x)|x)$, which are not the desired gradients. Note that we do not know the exact calculation rule of $\log q^\phi_{Z|X}(z|x)$ for arbitrary z and x, but can only evaluate $h^\phi(e, x) := \log q^\phi_{Z|X}(T_\phi(e|x)|x)$ from a given e and x. Automatic differentiation could only evaluate the gradients of this $h^\phi(e, x)$ but not of $\log q^\phi_{Z|X}(z|x)$.

Solution. An explicit deduction is thus required for an expression of the correct gradients in terms of what automatic differentiation could evaluate. From the chain rule, we have:

$$\nabla_e h^\phi(e, x) = \nabla_e \log q^\phi_{Z|X}(T_\phi(e|x)|x) = \big(\nabla_e T_\phi^\top(e|x)\big)\big(\nabla_Z \log q^\phi_{Z|X}(T_\phi(e|x)|x)\big),$$

[12]Although some flow-based models (*e.g.*, the Sylvester flow [59]) also incorporate the dependency on x in the base distribution $\tilde{p}_\phi(\tilde{e}|x)$ (*e.g.*, $\mathcal{N}(\tilde{e}|\mu_\phi(x), \Sigma_\phi(x))$), we can reparameterize this distribution as transformed from a "more basic" parameter-free base distribution $p(e)$ (*e.g.*, $\mathcal{N}(0, I_{d_\mathbb{Z}})$) by an x-dependent transformation (*e.g.*, $\tilde{e} = \mu_\phi(x) + \Sigma_\phi(x)^{1/2} e$) and concatenate this transformation to the original one as $z = T_\phi(e|x)$.

$$\nabla_x h^\phi(e,x) = \nabla_x \log q^\phi_{Z|X}(T_\phi(e|x)|x) = \big(\nabla_x T_\phi^\top(e|x)\big)\big(\nabla_Z \log q^\phi_{Z|X}(T_\phi(e|x)|x)\big) + \nabla_X \log q^\phi_{Z|X}(T_\phi(e|x)|x).$$

The first equation gives one of the desired gradients: $\nabla_Z \log q^\phi_{Z|X}(T_\phi(e|x)|x) = \big(\nabla_e T_\phi^\top(e|x)\big)^{-1}\big(\nabla_e h^\phi(e,x)\big)$. The term $\nabla_e h^\phi(e,x)$ can be evaluated using automatic differentiation, as mentioned. The other term, *i.e.* the Jacobian $\nabla_e T_\phi^\top(e|x)$, can also use automatic differentiation by tracking the forward flow computation $z = T_\phi(e|x)$, but it is often available in closed-form for flow-based models, as flow-based models need to evaluate its determinant anyway so the architecture is designed to give its closed-form expression.

The second equation gives an expression of the other desired gradient: $\nabla_X \log q^\phi_{Z|X}(T_\phi(e|x)|x) = \nabla_x h^\phi(e,x) - \big(\nabla_x T_\phi^\top(e|x)\big)\big(\nabla_Z \log q^\phi_{Z|X}(T_\phi(e|x)|x)\big)$. Again, the first term $\nabla_x h^\phi(e,x)$ can be evaluated using automatic differentiation. The term $\big(\nabla_Z \log q^\phi_{Z|X}(T_\phi(e|x)|x)\big)$ can be evaluated using the expression we just derived above. For the rest term, *i.e.* the Jacobian $\nabla_x T_\phi^\top(e|x)$, it can also be evaluated using automatic differentiation by tracking the forward flow computation $z = T_\phi(e|x)$. For computation efficiency, this can be implemented by taking the gradient of $z = T_\phi(e|x)$ w.r.t x with the `grad_outputs` argument of `torch.autograd.grad` fed by $\nabla_Z \log q^\phi_{Z|X}(T_\phi(e|x)|x)$ (gradients w.r.t x will not be back-propagated through this $\nabla_Z \log q^\phi_{Z|X}(T_\phi(e|x)|x)$). This reduces computation complexity from $O(d_{\mathbb{X}} d_{\mathbb{Z}})$ down to $O(d_{\mathbb{X}} + d_{\mathbb{Z}})$. In summary, the desired gradients can be computed via the following expressions:

$$\nabla_Z \log q^\phi_{Z|X}(T_\phi(e|x)|x) = \big(\nabla_e T_\phi^\top(e|x)\big)^{-1}\big(\nabla_e h^\phi(e,x)\big), \tag{20}$$

$$\nabla_X \log q^\phi_{Z|X}(T_\phi(e|x)|x) = \nabla_x h^\phi(e,x) - \big(\nabla_x T_\phi^\top(e|x)\big)\big(\nabla_Z \log q^\phi_{Z|X}(T_\phi(e|x)|x)\big). \tag{21}$$

Second-order differentiations for the compatibility loss can be done in a similar way.

A simplified compatibility loss. For the compatibility loss Eq. (3) in the form of Hutchinson's trace estimator, a further simplification is possible. The loss is given by:

$$C(\theta,\phi) = \mathbb{E}_{\rho(x,z)}\mathbb{E}_{p(\eta_x)}\Big\|\nabla_Z\big(\eta_x^\top \nabla_X \log p^\theta_{X|Z}(x|z) - \eta_x^\top \nabla_X \log q^\phi_{Z|X}(z|x)\big)\Big\|_2^2,$$

with any random vector η_x satisfying $\mathbb{E}[\eta_x] = 0, \mathrm{Var}[\eta_x] = I_{d_{\mathbb{X}}}$. The reference distribution $\rho(x,z)$ can be taken as $p^*(x)q_\phi(z|x)$ for practical sampling for estimating the expectation. For a flow-based $q_\phi(z|x)$, sampling from $(x,z) \sim p^*(x)q_\phi(z|x)$ is equivalent to $(x, T_\phi(e|x)), e \sim p(e)$. So the loss can be reformulated as:

$$C(\theta,\phi) = \mathbb{E}_{p^*(x)p(e)}\mathbb{E}_{p(\eta_x)}\Big\|\nabla_Z\big(\eta_x^\top \nabla_X \log p^\theta_{X|Z}(x|T_\phi(e|x)) - \eta_x^\top \nabla_X \log q^\phi_{Z|X}(T_\phi(e|x)|x)\big)\Big\|_2^2.$$

Note from Eq. (20), the gradient w.r.t Z is an invertible linear transformation of the gradient w.r.t e, so its norm equals zero if and only if the gradient w.r.t e has a zero norm. So to avoid this matrix inversion, we consider a simpler loss that achieves the same optimal solution:

$$\tilde{C}(\theta,\phi) := \mathbb{E}_{p^*(x)p(e)}\mathbb{E}_{p(\eta_x)}\Big\|\nabla_e\big(\eta_x^\top \nabla_X \log p^\theta_{X|Z}(x|T_\phi(e|x)) - \eta_x^\top \nabla_X \log q^\phi_{Z|X}(T_\phi(e|x)|x)\big)\Big\|_2^2. \tag{22}$$

For additive Gaussian $p^\theta_{X|Z}$, its gradient $\nabla_X \log p^\theta_{X|Z}$ is available in closed-form. For $\nabla_X \log q^\phi_{Z|X}(T_\phi(e|x)|x)$ in the second term, it can be estimated using Eq. (21) we just developed. The subsequent gradient w.r.t e can be evaluated by automatic differentiation. So this loss is tractable to estimate and optimize.

E Experiment Details

E.1 Baseline Methods

We compare our proposed CyGen with bi-directional training methods including Variational Auto-Encoder (VAE), Denoising Auto-Encoder (DAE) and BiGAN. Sketches of the aforementioned methods are presented as follows.

VAE [33] defines a joint distribution $p_\theta(x, z) = p(z)p_\theta(x|z)$ using a specified prior $p(z)$. It learns $p_\theta(x|z)$ to match data distribution $p^*(x)$ with the help of an inference model $q_\phi(z|x)$, using the Evidence Lower BOund (ELBO) objective:

$$\min_{\theta,\phi} \mathbb{E}_{p^*(x)}\mathbb{E}_{q_\phi(z|x)}\left[-\log p_\theta(x|z)\right] + \beta\mathbb{E}_{p^*(x)}[\mathrm{KL}(q_\phi(z|x)\|p(z))]. \tag{23}$$

When $\beta = 1$, the negative objective is a lower bound of the data likelihood (evidence) $\mathbb{E}_{p^*(x)}[\log p_\theta(x)]$ where $p_\theta(x) := \int_{\mathbb{Z}} p(z)p_\theta(x|z)\mathrm{d}z$, hence the name. Optimizing it w.r.t ϕ also drives $q_\phi(z|x)$ to the true posterior $p_\theta(z|x)$ and also makes the bound tighter. A β other than 1 is considered when there is some desideratum on the latent variable, *e.g.*, disentanglement [26].

DAE [61] first corrupts a real input data x with a local noise and then pass it through an encoder to define $q_\phi(z|x)$. The latent code z is then decoded to the data space by a decoder $p_\theta(x|z)$. The objective is to minimize the reconstruction error: $\mathbb{E}_{p^*(x)}\mathbb{E}_{q_\phi(z|x)}[-\log p_\theta(x|z)]$. Compared with VAE, it can be seen as the version with $\beta = 0$, *i.e.* it does not involve a prescribed prior $p(z)$. Nevertheless, optimizing the objective w.r.t ϕ may lead to undesired results. Particularly, for any given x, it may drive $q_\phi(z|x)$ to only concentrate on z values that maximizes $\log p_\theta(x|z)$. This renders incompatibility and an insufficient determinacy.

BiGAN [17, 18]. In addition to learning the data distribution $p^*(x)$ using GAN [21], BiGAN also aims to learn a representation extractor, so it introduces an inference model $q_\phi(z|x)$ which is often deterministic (*i.e.*, a Dirac distribution). The likelihood model (generator) $p_\theta(x|z)$ defines a joint $p(z)p_\theta(x|z)$ with the help of a prescribed prior $p(z)$, while the inference model also defines a joint $p^*(x)q_\phi(z|x)$. Samples from both distributions can be easily drawn, so BiGAN seeks to match them using the GAN loss (Jensen-Shannon divergence) with the help of a discriminator $D(x, z)$. In each training step, the discriminator $D(x, z)$ is first updated on a mini-batch of $p^*(x)q_\phi(z|x)$ data $x^+ \sim p^*(x), z^+ \sim q_\phi(\cdot|x^+)$ with positive labels $y^+ = 1$ and a mini-batch of $p(z)p_\theta(x|z)$ data $z^- \sim p(z), x^- \sim p_\theta(\cdot|z^-)$ with negative labels $y^- = 0$. The goal of the training the discriminator is to minimize the binary cross entropy loss $\mathrm{BCE}(D(x^+, z^+), y^+) + \mathrm{BCE}(D(x^-, z^-), y^-)$. The conditional models $q_\phi(z|x)$ and $p_\theta(x|z)$ are then updated to maximize the same loss $\mathrm{BCE}(D(x^+, z^+), y^+) + \mathrm{BCE}(D(x^-, z^-), y^-)$.

We also considered the GibbsNet [38] model, which is similar to BiGAN except that the prior-driven joint $z^- \sim p(z), x^- \sim p(x|z^-)$ involves running through multiple cycles, $z_0 \sim p(z), x_0 \sim p(x|z_0), z_1 \sim q(z|x_0), x_1 \sim p(x|z_1), \cdots, z^- \sim q(z|x_{K-1}), x^- \sim p(x|z^-)$. This resembles a Gibbs chain. But this iterated application of the encoder and decoder makes differentiation involved, and we did not find a reasonable result in any experiment under our choice of architecture. So we did not show the comparison with GibbsNet using the same architecture.

E.2 Model Structures

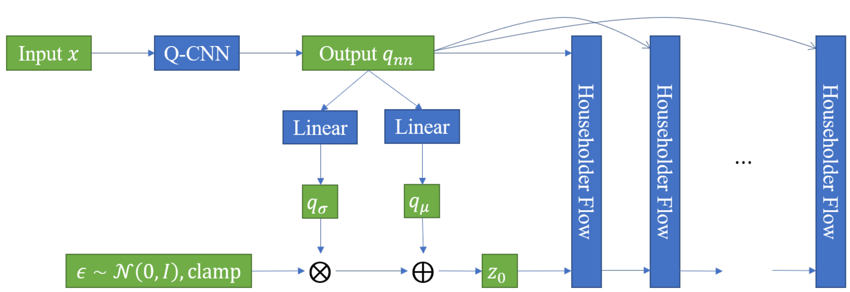


Figure 10: Flow architecture for the inference model $q_\phi(z|x)$.

Our code is developed based on the repository of Sylvester flow[13] [59] and FFJORD[14] [22] for the task environment and flow architectures. VAE, DAE and CyGen share the same architecture of $p_\theta(x|z)$ and of $q_\phi(z|x)$, which are detailed in Table 4. The inference model $q_\phi(z|x)$ adopts the architecture of Sylvester flow [59]. It consists of a neural network (denoted as C-QNN) that outputs q_{nn}, a reparameterization module, and a set of consecutive N flows. The outputs q_μ and q_σ are used to parameterize the diagonal Gaussian distribution for initializing z_0, the input to the flows. For

[13] `https://github.com/riannevdberg/sylvester-flows`

[14] `https://github.com/rtqichen/ffjord`

implementation simplicity, we choose the Householder version of the Sylvester flow. For each flow layer, the output $\mathbf{z}_t$ of the flow given input $\mathbf{z}_{t-1}$ is:

$$\mathbf{z}_t = \mathbf{z}_{t-1} + \mathbf{A}_t h(\mathbf{B}_t \mathbf{z}_{t-1} + \mathbf{b}_t),$$

where $\mathbf{A}_t = \mathbf{Q}_t \mathbf{R}_t$, $\mathbf{B}_t = \tilde{\mathbf{R}}_t \mathbf{Q}_t$ and $\mathbf{b}_t$ are parameters of the t-th flow and h is the hyperbolic-tangent activation function. Let $\mathbf{A} = \mathbf{Q}\mathbf{R}$, $\mathbf{B} = \tilde{\mathbf{R}}\mathbf{Q}^T$, where $\mathbf{R}$ and $\tilde{\mathbf{R}}$ are upper triangular matrices, and $\mathbf{Q} = \prod_{i=1}^{H}(\mathbf{I} - \frac{2\mathbf{v}_i\mathbf{v}_\mathrm{i}^\mathrm{T}}{\mathbf{v}_i^T\mathbf{v}_i})$ is a sequence of $H = 8$ Householder transformations. All the parameters of the flow $\mathbf{v}_{1:H}$, $\mathbf{R}$ and $\tilde{\mathbf{R}}$ depend on q_{nn}.

E.3 Synthetic Dataset

For experiments on synthetic dataset, the dimensions of x and z are both $d_\mathbb{X} = d_\mathbb{Z} = 2$. We use a three-layer MLP for modeling the C-QNN component, the number of hidden nodes in each layer is 8. After reparameterization, we use a consecutive of $N = 32$ Householder flow layers. Each flow has $H = 2$ Householder transformations[15]. The decoder $p_\theta(x|z)$ is implemented as an additive Gaussian model. Its mean function is a three-layer MLP with 16 hidden nodes on each layer. A fixed variance of 0.01 is used for the additive Gaussian noise.

We train both $p_\theta(x|z)$ and $q_\phi(z|x)$ of CyGen by choosing the weight of the compatibility loss (Eq. (3) or Eq. (22)) as $w_{\text{cm}} = 1\times10^{-5}$ (the weight of the data-fitting loss Eq. (4) is 1). We use the Adam optimizer [31] with step size 1×10^{-3}. For image generalization, we run Langevin dynamics on latent space using step size $\varepsilon = 3\times10^{-4}$.

For generation using VAE, samples from the isotropic Gaussian prior are passed through the likelihood model $p_\theta(x|z)$ to produce data samples. Generation using CyGen is done by passing through the likelihood model $p_\theta(x|z)$ with prior samples drawn via SGLD in the latent space $\mathbb{Z}$ similar to Eq. (5):

$$z^{(t+1)} = z^{(t)} + \varepsilon\nabla_{z^{(t)}} \log \frac{q_\phi(z^{(t)}|x^{(t)})}{p_\theta(x^{(t)}|z^{(t)})} + \sqrt{2\varepsilon}\eta_z^{(t)}, \text{where } x^{(t)} \sim p_\theta(x|z^{(t)}), \eta_z^{(t)} \sim \mathcal{N}(0, I_{d_\mathbb{Z}}), \quad (24)$$

and ε is a step size parameter.

Impact of the compatibility loss. We plot in Table 5 with samples generated from CyGen with and without compatibility loss along training. The two CyGen models are initialized identically by the $p_\theta(x|z)$ and $q_\phi(z|x)$ pretrained as a VAE, whose generation result is shown in the leftmost figure in Table 5. We see that the normal CyGen behaves stably and well approximates the data distribution along optimization, and the compatibility loss is decreasing. On the other hand, the CyGen without the compatibility loss diverges eventually, with an exploding compatibility loss. Although it well optimizes the data-fitting loss Eq. (4), if compatibility is not enforced, the loss is not the data likelihood that we want to optimize.

Note that the CyGen without compatibility loss improves the generation quality upon the VAE-pretrained model in the first few training iterations. This is because the ELBO objective (Eq. (23)) of VAE also drives $q_\phi(z|x)$ towards the true posterior $p_\theta(z|x) \propto p(z)p_\theta(x|z)$ so compatibility approximately holds in the first few iterations, which makes the data-fitting loss (Eq. (4)) effective.

Incorporating knowledge into the conditionals. We plot the prior distributions of VAE, CyGen without and with VAE pretraining in Fig. 11, in the form of the histogram of drawn samples. For CyGen models, samples are drawn by $\mathbb{Z}$-space SGLD. For the CyGen with VAE pretraining, $p_\theta(x|z)$ and $q_\phi(z|x)$ are first trained by minimizing the ELBO objective with the standard Gaussian prior, and are then trained by minimizing the CyGen objective (compatibility loss + data-fitting loss) with a 10-times smaller learning rate for $p_\theta(x|z)$. Compared to VAE, the priors learned by CyGen are more expressive. For CyGen without any further constraints, there may be multiple $p_\theta(x|z)$ and $q_\phi(z|x)$ that are compatible and match the given data distribution. The results in Fig. 11 show that using a standard Gaussian prior for pretraining successfully incorporates the knowledge of a centered and centrosymmetric prior into the conditional model $p_\theta(x|z)$, so the arbitrariness is greatly mitigated.

E.4 Real-World Datasets

All generative models share the same encoder (inference model) and decoder (likelihood model) architectures, except BiGAN and GibbsNet which did not show reasonable results using the same architecture. For the downstream classification task on the latent space, after training the generative

[15] To make an invertible transformation, the number of Householder transformations H needs to be no larger than the dimension of z, which is 2 in the synthetic experiment

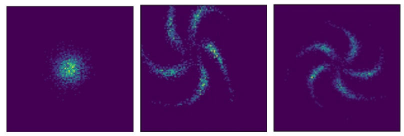


Figure 11: Prior distributions $p(z)$ of VAE (left), CyGen (without pretraining) (middle), and CyGen with VAE pretraining (right). Prior samples of CyGen models are drawn using $\mathbb{Z}$-space SGLD (Eq. (24)).

model, we sample the latent representation directly from the inference model $q_\phi(z|x)$, and then train a 2-layer MLP classifier with 10 hidden nodes on top of the latent representation. All generative models and the downstream classifiers are trained for 100 epochs.

E.4.1 MNIST

For experiments on SVHN, we pretrain the model using the standard ELBO in Eq. (23) with $\beta = 1$ for 100 epochs using Adam optimizer with learning rate 1×10^{-4}. The mini-batch size is 100. The test accuracy after pretraining is about 95%.

We then train both the encoder and decoder using CyGen by setting the weight of compatibility loss $w_{\text{cm}} = 1 \times 10^{-3}$. The variance of decoder $p_\theta(x|z)$ is selected to be 0.01, independent on each dimension. The learning rate for $q_\phi(z|x)$ and $p_\theta(x|z)$ are set to 1×10^{-4} and 1×10^{-5}, respectively. For image generation, first draw $z_0 \sim \mathcal{N}(0, \mathbf{I})$ and then obtain $x_0 \sim p_\theta(\cdot|z_0)$. Then we run Langevin dynamics on x using stepsize $\eta = 0.001$.

E.4.2 SVHN

For experiments on SVHN, we pretrain the model using VAE by choosing $\beta = 0.01$ for 100 epochs with Adam optimizer using learning rate 1×10^{-4} with mini-batch size $n = 100$. In reparameterization step, we clamp ϵ that initializes z_0 to interval $[-0.1, 0.1]$. The test accuracy after pretraining is about 75%. Hyperparameters for training CyGen and image generation are the same as on MNIST dataset.

Table 4: Encoder and decoder structures for MNIST and SVHN

Layers	In-Out Size	Stride
Encoder Structure $q_\phi(z\|x)$ **for MNIST**-C-QNN		
Input x	$1\times28\times28$	
5×5 GatedConv2d (32), Sigmoid	$32\times28\times28$	1
5×5 GatedConv2d (32), Sigmoid	$32\times14\times14$	2
5×5 GatedConv2d (64), Sigmoid	$64\times14\times14$	1
5×5 GatedConv2d (64), Sigmoid	$64\times7\times7$	2
5×5 GatedConv2d (64), Sigmoid	$64\times7\times7$	1
7×7 GatedConv2d (256), Sigmoid	$256\times1\times1$	1
Output q_{nn}, squeeze	256	
Encoder Structure $q_\phi(z\|x)$ **for SVHN**-C-QNN		
Input x	$3\times32\times32$	
5×5 Conv2d (32), LReLU	$32\times28\times28$	1
4×4 Conv2d (64), LReLU	$64\times13\times13$	2
4×4 Conv2d (128), LReLU	$128\times10\times10$	1
4×4 Conv2d (256), LReLU	$256\times4\times4$	2
4×4 Conv2d (512), LReLU	$512\times1\times1$	1
4×4 Conv2d (256), Sigmoid	$256\times1\times1$	1
Output q_{nn}, squeeze	256	
Reparameterization Block $q_\phi(z\|x)$ **for MNIST and SVHN**		
Input q_{nn}	256	
Output-1 q_μ: Linear 256×64	64	
Draw $\epsilon\sim\mathcal{N}(0,\mathbf{I})$ and output $z_0=q_\mu+\epsilon\odot q_\sigma$	64	
Flow Parameter Generation $q_\phi(z\|x)$ **for MNIST and SVHN**		
Input q_{nn}	256	
Output-1 $v_{1:8}$: Linear 256×512	512	
Output-2 b: Linear 256×8	512	
Output-3 $\mathbf{R}$: Linear $256\times(64\times64)$	(64×64)	
Output-4 $\tilde{\mathbf{R}}$: Linear $256\times(64\times64)$	(64×64)	
Decoder Structure $p_\theta(z\|x)$ **for MNIST**		
Input z	$64\times1\times1$	
7×7 GatedConvT2d (64), Sigmoid	$64\times7\times7$	1
5×5 GatedConvT2d (64), Sigmoid	$64\times7\times7$	1
5×5 GatedConvT2d (64), Sigmoid	$64\times14\times14$	2
5×5 GatedConvT2d (32), Sigmoid	$32\times14\times14$	1
5×5 GatedConvT2d (32), Sigmoid	$32\times28\times28$	2
5×5 GatedConvT2d (32), Sigmoid	$32\times28\times28$	1
1×1 GatedConv2d (1), Sigmoid	$1\times28\times28$	2
Output x	$1\times28\times28$	
Decoder Structure $p_\theta(z\|x)$ **for SVHN**		
Input z	$64\times1\times1$	
4×4 ConvT2d (256), LReLU	$256\times4\times4$	1
4×4 ConvT2d (128), LReLU	$128\times10\times10$	1
4×4 ConvT2d (64), LReLU	$64\times13\times13$	1
4×4 ConvT2d (32), LReLU	$32\times28\times28$	2
5×5 ConvT2d (32), LReLU	$32\times32\times32$	1
1×1 ConvT2d (32), LReLU	$32\times32\times32$	1
1×1 Conv2d (32), Sigmoid	$32\times32\times32$	1
Output x	$3\times32\times32$	

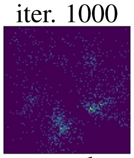
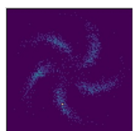
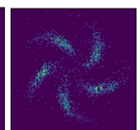
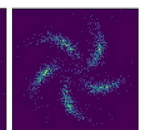
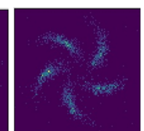
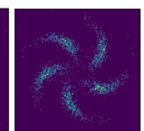
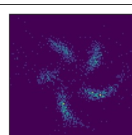
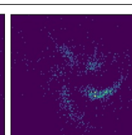
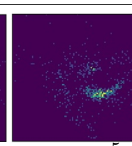
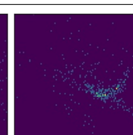
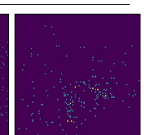
	iter.	1100	1200	1300	1400	30000
VAE pretraining iter. 1000 	CyGen					
compt. loss 1.6×10^4	compt. loss	7.0×10^3	5.4×10^3	7.7×10^3	6.2×10^3	4.6×10^3
	CyGen w/o compt. loss					
	compt. loss	1.1×10^5	1.6×10^5	2.6×10^5	8.6×10^5	1.2×10^8

Table 5: Generation qualities of CyGen (with compatibility loss weight $w_{\text{cm}} = 1\times10^{-5}$) and CyGen without compatibility loss after VAE pretraining. Data samples are generated by $\mathbb{Z}$-space SGLD (Eq. (24)) followed by passing through $p_\theta(x|z)$.