INDETERMINACY IN LATENT VARIABLE MODELS:  
CHARACTERIZATION AND STRONG IDENTIFIABILITY  

BY QUANHAN XI\textsuperscript{1,a} AND BENJAMIN BLOEM-REDDY\textsuperscript{1,b}  

\textsuperscript{1}Department of Statistics, University of British Columbia,  
a\texttt{johnny.xi@stat.ubc.ca}; \texttt{b}benbr@stat.ubc.ca  

Most modern latent variable and probabilistic generative models, such as the variational autoencoder (VAE), have certain indeterminacies that are unresolved even with an infinite amount of data. Recent applications of such models have indicated the need for strongly identifiable models, in which an observation corresponds to a unique latent code. Progress has been made towards reducing model indeterminacies while maintaining flexibility, most notably by the iVAE [19], which excludes many—but not all—indeterminacies. We construct a full theoretical framework for analyzing the indeterminacies of latent variable models, and characterize them precisely in terms of properties of the generator functions and the latent variable prior distributions. To illustrate, we apply the framework to better understand the structure of recent identifiability results. We then investigate how we might specify strongly identifiable latent variable models, and construct two such classes of models. One is a straightforward modification of iVAE; the other uses ideas from optimal transport and leads to novel models and connections to recent work.  

1. Introduction. It has long been known that even simple latent variable models like factor analysis and linear independent components analysis (ICA) are underdetermined, or unidentifiable, even with an infinite sequence of observations. In other words, not all aspects of those models can be inferred from empirical evidence, and further constraints in the form of assumptions or inductive biases must be imposed in order to resolve the underdetermination. Identifiability in latent variable models has been the subject of much recent work, motivated as a way to address a variety of problems ranging from disentanglement in representation learning [24, 10, 44, 22], posterior collapse [40], blind source separation [8], and causal representation learning [41, 36, 26]. One area within that literature relies on the identifiable variational autoencoder (iVAE) and its extensions [19, 20, 45, 28] which, building on results for nonlinear ICA [12, 13, 15, 10], guarantees under certain conditions that the latent code corresponding to an observation is uniquely identified up to some equivalence class—
the most precise of which are up to permutations and component-wise scalings. Other work [9, 25, 41, 1, 29, 43] has used apparently different techniques to establish identifiability of different latent variable models.

Although the identifiability results in recent work are stronger and apply to more flexible models than those previously known, they are still weak in the sense that they identify the model parameters and latent codes only up to non-trivial equivalence classes, often induced by unknown component-wise invertible mappings. Moreover, the techniques used to establish identifiability seem somewhat disparate and difficult to generalize. This motivates two questions:

1. Is there a common framework from which these different results can be obtained?
2. Are stronger identifiability results possible?

We answer both in the affirmative. We first establish a formal framework that yields a full characterization of the sources of indeterminacy (i.e., unidentifiability) in a general class of latent variable models, and show how identifiability results for factor analysis, ICA, iVAE, and others arise naturally within the framework. Our framework can be regarded as a general formal approach to characterizing latent variable model indeterminacies. Importantly, it cleanly separates the two sources of indeterminacy, which makes reasoning about how to eliminate them much more transparent. We then consider how we might obtain strong identifiability in latent variable models in the multiple environment setting, and obtain, to the best of our knowledge, the first strong latent variable identifiability result. Although it is obtained from a surprisingly simple modification of the iVAE, it is our framework that makes such a result apparent. We also consider an entirely different approach, again based on our framework, arriving at a novel class of models whose indeterminacies are measure transport maps, and obtain strong identifiability—even with a single environment—in a certain model sub-class.

1.1. Outline. In the rest of this section, we review two simple well-known examples in order to highlight the salient aspects of the problem, which generalize to more complex models. Section 2 contains the necessary definitions and assumptions. In Section 3, we construct the framework for analyzing the sources of indeterminacy in latent variable models, and present the main technical results. We apply the framework to analyze the multiple-environment setting in Section 4, showing in detail how recent work fits into the framework. In Section 5 we
describe indirect approaches to specifying strongly identifiable models based on (optimal) measure transports, and analyze particular versions based on the Knöthe–Rosenblatt and the Brenier transformations.

1.2. **Factor analysis and linear ICA.** We first review two well-known linear models to act as points of reference throughout the rest of the paper. The theory we develop is largely a generalization of the intuitive notions of unidentifiability in these simpler models, and we will often refer back to this section to ground our abstractions.

For observations modeled as random vectors \(X\) taking values in \(\mathbb{R}^{d_x}\), factor analysis [23] aims to infer a low-dimensional latent variable \(Z\) taking values in \(\mathbb{R}^{d_z}\), \(d_z < d_x\), via the model

\[
Z \sim \mathcal{N}(0, I_{d_z \times d_z}), \quad \epsilon \sim \mathcal{N}(\mu, I_{d_x \times d_x}), \quad X = FZ + \epsilon,
\]

where \(\epsilon_i\) is independent of \(Z_i\), and \(F\) is a full-rank \(d_x \times d_z\) matrix of so-called factor loadings, to be learned from data. We can think of this as structurally identical to a linear VAE. It is well known that the parameter \(F\) and the latent variables corresponding to the observations are unidentifiable: a single marginal distribution on \(X\) may correspond to (at least) two different factor loading matrices, say \(F_a\) and \(F_b\). To see this, note that Gaussian additive noise can be deconvolved [27], so the distribution of \(X\) is entirely determined by the distribution of \(FZ\).

Let \(F_b = F_aA_{a,b}\), with \(A_{a,b}\) some \(d_z \times d_z\) matrix. Since \(Z\) is a standard multivariate Gaussian, \(F_aZ \sim \mathcal{N}(0, F_aF_a^\top)\) and \(F_aA_{a,b}Z \sim \mathcal{N}(0, F_aA_{a,b}A_{a,b}^\top F_a^\top)\), and \(F_aZ \overset{d}{=} F_aA_{a,b}Z \overset{d}{=} F_bZ\) if and only if \(A_{a,b}A_{a,b}^\top = I_{d_z \times d_z}\). That is, the corresponding indeterminacy set consists of the set of \(d_z \times d_z\) orthogonal matrices. Another way of characterizing the indeterminacies, consistent with the framework we develop in Section 3, is to note that when \(A_{a,b}\) is an orthogonal matrix, \(A_{a,b}Z \overset{d}{=} Z\). That is, it preserves the latent variable distribution. Moreover, it can be constructed as \(A_{a,b} = F_a^{-1}F_b\), \(^1\) for two factor loading matrices in the model class. As we will show, generalizations of those are precisely the two conditions that characterize indeterminacies in more general models.

Linear ICA [5] relaxes the assumption that \(Z\) has a normal distribution, and only requires that the components of \(Z\) are independent. Typically, an ICA model is specified with a class of distributions on \(Z\), denoted \(\mathcal{P}_z\). The so-called mixing function, \(F\), and \(P_z \in \mathcal{P}_z\) are then inferred simultaneously from data. The indeterminacies of this model arise as any full-rank

---

\(^1\)Technically, this is the left-inverse of \(F_a\); see Appendix D.
matrix $A_{a,b}$ such that $F_a A_{a,b} Z_a \overset{\text{def}}{=} F_b Z_b$, where the indices $a$ and $b$ represent latent variables with different distributions in $\mathcal{P}_z$. The indeterminacy set now includes certain unresolvable ambiguities that arise from $A_{a,b}$ transporting the distribution of $Z_a$ to that of $Z_b$, in addition to the measure preserving transformations in the previous example. In particular, $Z_a$ and $Z_b$ may be a permutation and scaling of each other. If $\mathcal{P}_z$ excludes Gaussian distributions, it is known that these are the only two types of transformations in the indeterminacy set for linear ICA \cite{5}. On the other hand, in nonlinear ICA, many more indeterminacies may arise because $A_{a,b}$ does not need to be linear.

These examples illustrate that model indeterminacies come not only from the distribution(s) on $Z$, but also how they interact with the class of functions mapping the latent variables into the observation space. We make this precise in the next two sections.

2. Identifiability in latent variable models. Conceptually, our results are relatively simple, though some care is required to establish them rigorously. We have chosen to develop the ideas in the main text within a mathematical framework, with intuitive explanations when possible. The factor analysis and linear ICA examples serve as intuitive reference points. See Appendix A for a brief technical background. All proofs not included in the main text can be found in Appendix B.

A Borel space $(X, \mathcal{B}(X))$ is a topological space $X$ equipped with the $\sigma$-algebra generated by its open sets, denoted $\mathcal{B}(X)$. All spaces in this paper will be Borel spaces, and for convenience we leave the $\sigma$-algebra implicit in the notation, referring to the Borel space $(X, \mathcal{B}(X))$ simply as $X$. Let $Z$ and $X$ be two Borel spaces and $f: Z \to X$ a measurable function. If $f$ is bijective and bi-measurable (i.e., the inverse is also measurable) then it is called a Borel isomorphism of $Z$ and $X$. If $X = Z$ then $f$ is a Borel automorphism. If two probability measures $\mu$ and $\nu$ are defined on $Z$ and $X$, respectively, a Borel isomorphism $f$ is also a $(\mu, \nu)$-measure isomorphism if $\mu = \nu \circ f^{-1}$ and $\nu = \mu \circ f$. A Borel automorphism $f$ is also a $\mu$-measure automorphism if $\mu = \mu \circ f^{-1} = \mu \circ f$.\footnote{\(\mu \circ f^{-1}\) is the image measure, also known as the pushforward, and sometimes denoted by $f_\# \nu$ or $f_* \nu$.}

Throughout, we will use the notation $X$ and $Z$ for Borel spaces representing the observable space and latent space, respectively. In practice, typically $X = \mathbb{R}^{d_x}$ and $Z = \mathbb{R}^{d_z}$, $d_z \leq d_x$. 


For clarity, we will typically refer to these specific Borel spaces, but our framework applies
to general Borel spaces.

2.1. Model definition. Suppose that we model observations denoted \( x_i \) as i.i.d. realiza-
tions of a random variable \( X \) with distribution \( P_x \) on \( X \). Define a latent random variable
\( Z \) with corresponding realizations \( z_i \), with distribution \( P_z \) on the latent space \( Z \). We further
assume the presence of some noise realization \( \epsilon_i \), with some distribution \( P_\epsilon \) on some measur-
able space. Let \( f : Z \to X \) be a measurable function, which we call the generator. We define
a generative model as,

\[
Z \sim P_z, \quad \epsilon \sim P_\epsilon, \quad Z \perp \perp \epsilon, \quad \text{and} \quad X = g(f(Z), \epsilon).
\]

(2)

In words, a generator \( f \) maps a realization of the latent variable to a noiseless observation,
while \( g \) is a noise mechanism that corrupts the observation. For example, in a VAE or factor
analysis, \( X \) and \( Z \) are Euclidean spaces, and \( g(f(z), \epsilon) = f(z) + \epsilon \) is additive noise. In this
article, we will not be concerned with inferring the noise. Instead, we will work with the
assumption that the noise distribution and mechanism are fixed and have null effect on the
probabilistic properties of the model.

ASSUMPTION 1. Assume that \( g \) and \( P_\epsilon \) are such that \( g(f(Z_a), \epsilon_a) \overset{d}{=} g(f(Z_b), \epsilon_b) \), with
\( \epsilon_a \overset{d}{=} \epsilon_b \), if and only if \( f(Z_a) \overset{d}{=} f(Z_b) \).

This assumption includes for example the noiseless case, and additive noise for a suitable
noise distribution (see [10], for example). It means that, for identifiability purposes, it is
sufficient to analyze the noiseless case. We note that it rules out the possibility of discrete
observations except in very limited cases; see Section 6 for a brief discussion of this point.
For technical reasons, we will also assume that the generators are bijective on their range;
this is standard in the ICA literature.

ASSUMPTION 2. Assume that any \( f \in \mathcal{F} \) is injective, and has the same image: for any
\( f_a, f_b \in \mathcal{F}, f_a(Z) = f_b(Z) := \mathcal{F}(Z) \subseteq X \).

This assumption is necessary for making the inverse problem of recovering latents well-
defined. For example, the full rank matrices in linear ICA, as well as bijective conformal
maps in the initial analysis of non-linear ICA [14].
2.2. Identifiability. With Assumptions 1 and 2, designing a generative model involves specifying parameter spaces for the generator and the prior. We denote these as $\mathcal{F}$, a set of measurable functions from $\mathbb{Z} \to \mathbb{X}$; and $\mathcal{P}_z$, a set of probability measures on $\mathbb{Z}$. In the linear examples in Section 1.2, $\mathcal{F}$ consists of full-rank matrices; for factor analysis, $\mathcal{P}_z$ is the singleton $\{\mathcal{N}(0, I)\}$, and for ICA $\mathcal{P}_z$ is the set of distributions that factorize over the components of $Z$. For technical reasons, we also require a reference measure $\mu_z$ on $\mathbb{Z}$, relative to which densities and properties that hold ‘almost everywhere’ are defined. For $\mathbb{Z} = \mathbb{R}^d$, the natural reference measure is Lebesgue measure, denoted by $\lambda_z$.

A generative model induces as a statistical model for the observed data as

$$\mathcal{M}(\mathcal{F}, \mathcal{P}_z, \mu_z) = \{P_\theta \text{ on } \mathbb{X} \mid \theta = (f, \mathcal{P}_z), f \in \mathcal{F}, \mathcal{P}_z \in \mathcal{P}_z\}.$$  

Classically, a statistical model is called (strongly) identifiable if the mapping $\theta \mapsto P_\theta$ is one-to-one. We will work with an alternative definition, focusing on the generator and latent variable recovery.

**Definition 1.** The indeterminacy set of a model $\mathcal{M}(\mathcal{F}, \mathcal{P}_z, \mu_z)$, denoted $\mathcal{A}(\mathcal{M})$, is the set of bijectively measurable transformations $A: \mathbb{Z} \to \mathbb{Z}$ such that

$$P_{\theta_a} = P_{\theta_b} \iff f_a(z) = f_b(A(z)) \text{ for } \mu_z\text{-almost all } z \in \mathbb{Z}, \text{ for some } A \in \mathcal{A}(\mathcal{M}).$$

For the purposes of identifiability, we consider two functions equivalent if they are equal $\mu_z$-almost everywhere. This defines a proper equivalence relation [33]. In particular, let $\tilde{\text{id}}_z$ denote the class of functions that are equivalent to the identity mapping on $\mathbb{Z}$, $\text{id}_z$.

**Definition 2.** A generative model $\mathcal{M}(\mathcal{F}, \mathcal{P}_z, \mu_z)$ is weakly identifiable up to $\mathcal{A}(\mathcal{M})$, or $\mathcal{A}(\mathcal{M})$-identifiable, if its indeterminacy set is $\mathcal{A}(\mathcal{M})$. If $\mathcal{A}(\mathcal{M}) = \tilde{\text{id}}_z$, then the model is strongly identifiable.

Note that when the generator is parametrized via deep neural networks, the identifiability above does not necessarily pass to the learned weights and biases of the neural network. Rather, we use this point-wise definition merely as a proxy to make the notion of latent variable recoverability precise. In particular, because $f \in \mathcal{F}$ and $A \in \mathcal{A}(\mathcal{M})$ are bijective by definition, if two latent values $z_a, z_b$ generate the same observation $x$ in an $\mathcal{A}(\mathcal{M})$-identifiable model, then we must have $z_a = A(z_b)$. Similarly, $z_b = A^{-1}(z_a)$. In particular, if the model is
strongly identifiable, then we have $z_a = z_b$, and the generating latent variable is unique and hence recoverable.

We note here that any notion of model identifiability is an asymptotic property not achieved in practice. Even if there exists a unique latent variable that is in theory recoverable, there is no guarantee that a training algorithm will reach it with finite data. However, model identifiability is an important quality for statistical inference, and in particular is necessary for the typical theoretical guarantees [39]. Though future work is required to assess the finite-sample properties of strongly identifiable models, we remark that there is empirical evidence that even weak identifiability can recover latent structures that faithfully represent the ground truth [19, 37, 26].

3. Indeterminacy maps and characterizing identifiability. Our goal is to characterize precisely the class $A(M)$ for any model in the form of (2) satisfying Assumptions 1 and 2. Recall that by Assumption 2, all generators $f \in \mathcal{F}$ are bijective, and hence the inverse $f^{-1} : \mathcal{F}(Z) \to Z$ is well defined. The indeterminacy of the model for two generators $f_a$ and $f_b$ can be described by “pushing forward” and “pulling back” along these functions,

$$A_{a,b}(z) = f_b^{-1}(f_a(z)).$$

We refer to $A_{a,b} : Z \to Z$ as the indeterminacy map between $f_a$ and $f_b$, since clearly we have $f_a(z) = f_b(A_{a,b}(z))$, and for any observation $x_i$, a generating latent value $z_i$ through $f_a$ has an equally valid counterpart $z_i^* = A_{a,b}(z_i)$ through $f_b$. Being the composition of bijective functions, $A_{a,b}$ is clearly bijective. It can also be shown to be bijectively measurable (Lemma B.2)—in other words, $A_{a,b}$ is guaranteed to be a Borel automorphism of $Z$. Our first result states that it is also a measure isomorphism between two latent variable distributions if and only if the marginal distributions $P_{\theta_a}$ and $P_{\theta_b}$ agree.

**Lemma 3.1.** Let $\theta_a = (P_{z,a}, f_a)$ and $\theta_b = (P_{z,b}, f_b)$ be two parametrizations of a generative model with resulting marginal distributions $P_{\theta_a}$ and $P_{\theta_b}$. Then, $P_{\theta_a} = P_{\theta_b}$ if and only if $P_{z,b} = P_{z,a} \circ A_{a,b}^{-1}$ and $P_{z,a} = P_{z,b} \circ A_{a,b}$, where $A_{a,b}$ is the indeterminacy map (5).

Lemma 3.1 is the foundation for the rest of the paper, and can be interpreted as follows. Two parametrizations $\theta_a$ and $\theta_b$ induce the same element of the marginal model $\mathcal{M}$ if and only if we can transport between the two latent measures in $P_z$ by pushing and pulling along
Fig 1: Schematic representation of Lemma 3.1 for (a) measure isomorphisms (when \( P_z \) contains multiple elements); and (b) measure automorphisms (when \( P_z \) is a singleton).

the generators through \( A_{a,b} \). These are the scaling and permutation matrices in the linear ICA example from Section 1.2. When \( P_z \) is a singleton as in factor analysis, the measure isomorphism is a measure *automorphism*, such as the rotation matrices, which preserve the isotropic Gaussian distribution. See Figure 1 for a schematic visualization.

3.1. Indeterminacy sets. Lemma 3.1 gives a necessary and sufficient condition for two parameterizations to correspond to the same marginal distribution on observations. Though the “only if” may seem irrelevant at first glance, it also documents the cases in which \( P_\theta_a \) cannot be equal to \( P_\theta_b \), where identifiability may become strong. It allows us to construct exactly the set of model indeterminacies \( A(M) \) from indeterminacies generated by \( F \) and \( P_z \). To that end, define the sets of mappings induced by the generative model parameter spaces,

\[
A(F) = \{ A : Z \rightarrow Z \mid A = f_b^{-1} \circ f_a \text{ for some } f_a, f_b \in F \}
\]

\[
A(P_z) = \{ A : Z \rightarrow Z \mid P_b = P_a \circ A^{-1}, P_a = P_b \circ A \text{ for some } P_a, P_b \in P_z \}.
\]

\( A(F) \) consists of all possible indeterminacy maps constructed from \( F \), and \( A(P_z) \) consists of all possible isomorphisms between measures in \( P_z \). Both sets always include the identity function by taking \( f_a = f_b \) and \( P_a = P_b \). Lemma 3.1 implies that the indeterminacies of the model are precisely their intersection.

**Theorem 3.2.** *The generative model* \( M(F, P_z, \mu_z) \) *is identifiable up to* \( A(M) = A(F) \cap A(P_z) \). *In particular,* \( M(F, P_z, \mu_z) \) *is strongly identifiable if and only if* \( A(F) \cap A(P_z) = \tilde{id}_z \).
This expresses the identifiability of a generative model in terms of indeterminacy maps induced by its parameter spaces. In particular, all model indeterminacies must be transports between distributions in $\mathcal{P}_z$ that can be constructed by pushing and pulling along generators from $\mathcal{F}$ as $f_b^{-1} \circ f_a$. It suggests that the model identifiability strengthens as we increase the number of constraints on $\mathcal{F}$, $\mathcal{P}_z$, or both, until the intersection $\mathcal{A}(\mathcal{F}) \cap \mathcal{A}(\mathcal{P}_z)$ contains only the identity and strong identifiability is obtained. This approach to designing identifiable models is most clearly demonstrated in linear, non-Gaussian ICA: the linear constraint on $\mathcal{F}$ reduces indeterminacy maps to linear maps, and the non-Gaussianity in $\mathcal{P}_z$ is designed precisely to eliminate linearly isomorphic measures.

Theorem 3.2 exposes the structure of unidentifiability and indicates that there may be approaches to specifying strongly identifiable latent variable models without restricting ourselves to linear generators. The rest of the paper explores two such approaches. The first, in Section 4, uses multiple environments to impose additional constraints on the model. This is the approach used by iVAE and related models. The second approach, in Section 5, specifies $\mathcal{F}$ indirectly by restricting the indeterminacy maps in $\mathcal{A}(\mathcal{F})$ to satisfy specific properties.

4. Generative models in multiple environments. Suppose data arise from environments indexed by $e \in E$, where the environment label is assumed to be deterministic (i.e., known, or observed without noise). Each environment corresponds to a different observation random variable $X^e \sim P^e_x$ on a shared observation space $\mathbf{X}$. This is reflected in the generative model as $|E|$ distinct distributions on latent variables, $Z^e \sim P^e_z$ on a shared latent space $\mathbf{Z}$. Crucially, each environment shares the same generator $f$. The parameter space is $(\mathcal{F}, \{P^e_z\}_{e \in E})$, and the generative model is specified as, for each $e \in E$,

$$
Z^e \sim P^e_z, \quad \epsilon \sim P_{\epsilon}, \quad Z^e \perp \perp \epsilon, \quad \text{and} \quad X^e = g(f(Z^e), \epsilon_i).
$$

This setting is common in causal inference, where environments correspond to observational and interventional distributions [e.g., 32, 4]. There, relationships that are modular, or invariant across environments, are interpreted as more likely to be causal. Similar models have also been considered for out-of-distribution generalization, particularly under covariate shift [3, 26].

With multiple environments, identifiability as in (4) must hold simultaneously for each environment. Specifically, the definition of indeterminacy set (Definition 1) is extended so
that (4) becomes
\[ P_\theta^e = P_\theta^b \forall e \in E \iff f_a(z) = f_b(A(z)) \text{ for } \mu_z\text{-almost all } z \in Z, \text{ for some } A \in A(M). \]

Weak and strong identifiability remain as in Definition 2, with the multiple-environment indeterminacy set. Since the generator and hence the indeterminacy maps do not change across environments, Theorem 3.2 applies in each environment.

**Corollary 4.1.** The generative model \( M(\mathcal{F}, \{P_\theta^e\}_{e \in E}; \mu_z) \) is identifiable up to
\[ A(\mathcal{F}) \cap \left( \bigcap_{e \in E} A(P_\theta^e) \right). \]

We note that permutations of the environments are ruled out because the environments are assumed to be known. Clearly, the indeterminacy set shrinks with each environment added. As a demonstration of our framework we strengthen two recent identifiability results that can be re-framed as using multiple environments to constrain the indeterminacy set.

**4.1. Application to recent works.** Corollary 4.1 can be used to recover several identifiability results from recent literature. We detail a few examples below.

**4.1.1. Equivariant Stochastic Mechanisms.** In [1], weak identifiability of the following noiseless generative model is established, adapted to our notation:
\[
X_t = f(Z_t), \quad Z_{t+1} = m_t(Z_t, U_t), Z_t \perp U_t, \quad t = 1, 2, \ldots,
\]
where \( m_t \in M \) is an unknown mechanism. Denote the marginal distribution of \( Z_t \) as \( P_t \), and assume the initial condition \( Z_1 \sim P_1 \) for some fixed \( P_1 \) and \( U_t \sim U[0,1] \). Note the time indices here represent environments (we only require two “environments” \( t = 1, 2 \) to obtain the result).

In [1], identifiability of the generator \( f \) is established up to pre-composition of some transformation \( A \) such that \( A \circ m_a(z, U) \overset{d}{=} m_b(A(z), U) \) for \( U \sim U[0,1] \), for all possible values of \( z \), and \( m_a, m_b \in M \). Using our framework, we are able to show the following stronger identifiability result.

**Proposition 4.2.** The model described by (9) is identifiable up to \( A \in A(M) \) satisfying
\[
A(m_a(Z, U)) \overset{d}{=} m_b(A(Z), U),
\]
for any \( m_a, m_b \in M, U \sim U[0,1] \) and any random variable \( Z \) independent of \( U \).
Letting $P_1$ be any point mass recovers the original identifiability result in [1]. Our proof structure follow the intuition originally laid out in [1], but we do not assume a diffeomorphic generator, with the problem being formulated purely in measure theoretic terms.

4.1.2. **Identifiable VAE (iVAE).** In the iVAE model [19], the latent variable distribution varies via an auxiliary variable $u$ that indexes the environment. For simplicity, assume that $u$ is deterministic, e.g., a time index as suggested in [15, 19]. The latent distribution is parameterized as an exponential family distribution on $Z = \mathbb{R}^d$,

$$p(z; \eta(u)) = m(z) \exp(\eta(u)^\top T(z) - a(\eta(u))), \quad (11)$$

with functional parameters $\eta$, $T$ taking values in $\mathbb{R}^K$. Note that this means the latent distribution is inferred from data, as in non-linear ICA. The remainder of the model design follows (8) with additive noise. We note that in [19], the distribution is assumed to factorize over dimensions of $Z$ (as in ICA), but that is not necessary, an observation also made recently in [26].

In proving identifiability, iVAE requires the existence of points $u_0, u_1, \ldots$ such that $\eta(u_i) - \eta(u_0)$ are linearly independent and span the latent space. They are able to obtain that for parametrizations $(f_a, T_a, \eta_a)$ and $(f_b, T_b, \eta_b)$, there exists an invertible matrix $L$ and offset vector $c$ such that for all $x$,

$$T_a(f_a^{-1}(x)) = L^\top T_b(f_b^{-1}(x)) + c. \quad (12)$$

The above is the content of Theorem 1 of [19]. Using our framework, we are arrive at a similar result. Although we use similar arguments to those originally presented in [19], the indeterminacy set framework also sheds light on why the iVAE indeterminacies are of the particular form (12).

Suppose we have two sets of size $K + 1$ exponential family distributions, $a$ and $b$, each of which have linearly independent natural parameters. Proposition B.8 in the appendix shows that if a measure isomorphism $A$ transports the set of distributions $a$ to the set $b$, then $A$ must satisfy a version of (12) (see (13) below). These simultaneous transports are the indeterminacy maps. The following version of Theorem 1 from [19] is slightly stronger in that it does not require $f$ or $T$ to be differentiable.\(^3\)

---

\(^3\)We are unable to recover the stronger identifiability results of Theorems 2 and beyond in [19] without assuming $f$ to be a diffeomorphism because those proofs continue by analyzing $A_{a,b}$ and its partial derivatives.
PROP OS IT ION 4.3. Suppose a generative model is described by (8) with latent distributions described by (11), and that m is strictly positive. Suppose we observe at least K + 1 distinct values of \( u_i \) such that the corresponding natural parameters \( \{\eta(u_i)\}_{i=0}^{K} \) are linearly independent. Then, the indeterminacy map satisfies

\[
T_b(A_{a,b}(z)) = L^\top T_a(z) + d,
\]

\( \lambda_z \)-almost everywhere, where \( L \) is an invertible \( K \times K \) matrix and \( d \) is a \( K \)-dimensional vector.

4.2. Fixed versus learned latent distributions. As the previous discussion of the weak identifiability in iVAE (13) highlights, the indeterminacy stems from the possibility of simultaneously transporting the environment latent distributions to another set of distributions that are also contained in \( \mathcal{P}_z \). It is not apparent to us that that source of indeterminacies can be addressed without either: (i) fixing the latent distributions before fitting the generator; or (ii) cleverly constructing \( \mathcal{F}, \mathcal{P}_z \) to ensure that any indeterminacy map \( f^{-1}_b \circ f_a \) applied to any \( P_z \in \mathcal{P}_z \) transports \( P_z \) to a distribution not contained in \( \mathcal{P}_z \). The latter seems difficult to do in a flexible and general way, though it poses an interesting question for future research. Fixing the latent distributions, on the other hand, is easy, but it comes with questions about flexibility and interpretation. We briefly discuss these here, but substantial work is required to complete the picture.

From a philosophical perspective, without auxiliary information about the environments, there does not seem to be a good reason for not fixing the latent distributions, since even infinite data cannot resolve the model indeterminacies. Nothing in the data privileges one set of latent distributions over another if they lead to the same distribution on observations. The trend in recent years has been to let the data determine as many aspects of the model as possible, and one apparent cost of such an approach is a certain loss of control over the learned representations of observed data. For purely predictive purposes, this may not cost much; for modeling applications in which we wish to interpret or manipulate the learned representations, it is apparent that the models must strike a careful balance between flexibility and usability.

Fixing the latent distributions before fitting the generator is one way to achieve that balance, though how the distributions ought to be specified depends on the desired use of the
model, and the framework for doing so remains unresolved. The use of auxiliary data, for example the $u$ variables in iVAE, appear to be a useful and justifiable way to structure the latent space. In all of the “fixed latent distribution” identifiability results in the following sections, a mapping $u \mapsto P_z(u)$ can be learned from data (as in iVAE), as long as it is frozen at some point during training. This could be, for example, jointly learning $P_z(u)$ and $f$ for some number of training steps, after which $P_z(u)$ is fixed and $f$ is continued to be learned—though the justification for doing so is not apparent to us. More simply, the model could be trained in two steps: first $u \mapsto P_z(u)$ is learned via, for example, contrastive learning, and then $f$ is learned. We leave a full study of these topics for future work.

4.3. Strongly identifiable VAE with fixed latent distributions. In this section, we show an example of how fixed latent distributions, i.e., nonlinear factor analysis-type models can lead to strong identifiability. According to Theorem 3.2, with fixed latent distributions, the indeterminacy set is no larger than the set of measure preserving automorphisms of the latent space. However, constructing distributions such that the only automorphism is the identity is in general very difficult—non-trivial measure automorphisms, such as via the Darmois construction, can almost always be constructed (see [8] for an example). On the other hand, we show a very simple solution to this problem in multiple environments. It is essentially an adjustment of the iVAE for strong identifiability, with fixed latent distributions.

We assume the same setting as iVAE, with latent space $\mathbb{R}^{d_z}$ and natural parameter space $\mathbb{R}^K$. We denote a fixed set of full-rank exponential family distributions parameterized by $\eta$, by

$$\mathcal{E}_{m,T} = \{ P \text{ on } \mathbb{Z} \mid p(z; \eta) = m(z) \exp(\eta^T T(z) - a(\eta)); \eta \in \mathbb{R}^K \}.$$  \hspace{1cm} (14)

We refer to a particular distribution in a fixed family as $\mathcal{E}_{m,T}(\eta)$.

Proposition B.11 in the appendix states that the only shared automorphism for each distribution from a suitably fixed exponential family whose parameters form a basis of $\mathbb{R}^K$ is the identity. Strong identifiability follows when these are fixed as the latent distributions.

**Theorem 4.4.** Let $\mathcal{M}(\mathcal{F}, \{P^e_z\}_{e \in E}, \lambda_z)$ be the multiple environments model described in (8), with $Z = \mathbb{R}^{d_z}$. For a subset of environments $E^* \subset E$, with $|E^*| = K + 1$, fix $P^e_z = \mathcal{E}_{m,T}(\eta_e)$ with $m$ strictly positive and $T$ injective in at least one dimension, and such
that the corresponding parameters \( \{ \eta_e \}_{e \in E^*} \) span \( \mathbb{R}^K \). Then \( \mathcal{M}(\mathcal{F}, \{ P_e \}_{e \in E}, \lambda) \) is strongly identifiable.

The conditions of the theorem are met by \( d_z + 1 \) Gaussian distributions with standard covariance such that their means \( \mu_i, i = 0, 1, \ldots, d_z \) span \( \mathbb{R}^d \). More generally, injectivity of \( T \) is guaranteed so long as one of its dimensions is the identity (corresponding to a “Gaussian” dimension). Note the observation space remains an arbitrary Borel space of the same cardinality of \( \mathbb{R} \)—in particular, it may be bounded, such as \([0, 1]^m\).

We remark that if \( |E^*| < |E| \), the latent distributions for the remaining environments \( E \setminus E^* \) have no constraints; they do not need to be exponential family distributions and do not even need to be fixed. They may be fully flexible, and can be learned from data as in nonlinear ICA or iVAE.

We can characterize the indeterminacy set geometrically in terms of the orthogonal complements of the subspace spanned by the natural parameter vectors. This perspective is especially useful when considering the simple latent geometry of Gaussian distributions with environment-specific means: for a specific collection of Gaussian environments not necessarily spanning the entire space, the generative model is identifiable up to arbitrary transformations on the dimensions not spanned by the environment means. See Appendix B.4 for details.

5. Generative models specified with transport indeterminacies. In Section 4.3, \( \mathcal{F} \) was left unconstrained; strong identifiability was achieved through multiple environments and restricting the environment latent variable distributions to be fixed members of an exponential family distribution. In this section we construct models in which the latent variable distributions can by any fixed distributions with strictly positive density with respect to \( \lambda_z \) (denoted \( P_z \ll \lambda_z \)), and observations possibly from a single environment. This is achieved by restricting the class of generators, and with the additional condition that \( Z = X = \mathbb{R}^d \).

We approach the identifiability problem indirectly, by considering what properties of \( \mathcal{A}(\mathcal{F}) \) would yield strong identifiability. We aim to specify \( \mathcal{F} \) such that when \( A_{a,b} = f_b^{-1} \circ f_a \) transports one latent distribution to another, it is unique in a suitable sense so that, in particular, when it transports a distribution to itself, it must be (equivalent to) the identity map. To il-
Illustrate, we describe a general approach and give a specific example. As in Section 4.3, the results require the latent distribution(s) to be fixed, and the discussion in Section 4.2 applies.

5.1. Transport indeterminacies. Given two probability measures $P_a$ and $P_b$ on $\mathbb{R}^d$, the Monge formulation of optimal transport \cite{34} with respect to the cost function $c: \mathbb{Z} \times \mathbb{Z} \to \mathbb{R}_+$ is to find a map $T: \mathbb{Z} \to \mathbb{Z}$ such that $P_a \circ T^{-1} = P_b$ and that minimizes the total cost

\begin{equation}
\int_{\mathbb{R}^d} c(z, T(z)) dP_a(z).
\end{equation}

We call $T$ an optimal transport (OT) map with respect to $c$ if it minimizes (15) for transporting between some pair of probability distributions on $\mathbb{R}^d$. Let $T_c$ be the set of OT maps with respect to a cost $c$. Clearly, if $c$ is such that $c(z_1, z_2) = 0 \iff z_1 = z_2$, then the unique OT map from a distribution $P_z$ to itself is equal to the identity map $P_z$-almost everywhere. Because of the indeterminacy set framework and Theorem 3.2, the proof of the following result is trivial.

**Theorem 5.1.** Let $\mathbf{Z} = \mathbf{X} = \mathbb{R}^d$, and $P_z^e = \{P_z^e\}$, where for each $e \in E$, $P_z^e \ll \lambda_z$ is any fixed probability distribution on $\mathbb{R}^d$ with strictly positive density. If $A(F) \subseteq T_c$ for a cost satisfying $c(z_1, z_2) = 0 \iff z_1 = z_2$, then $M(F, \{P_z^e\}_{e \in E}, \lambda_z)$ is strongly identifiable for any $|E| \geq 1$.

**Proof.** By Theorem 3.2, the indeterminacy set $A(M) = A(F) \cap A(P_z) \subseteq T_c \cap A(P_z)$. Since $A(P_z)$ is the set of measure preserving automorphisms of $P_z$, its intersection with the optimal transport maps $T_c$ is equal to the identity $P_z$-almost everywhere. Since $P_z$ is fully supported on $\mathbb{R}^d$, $A(M)$ consists of maps equal to the identity almost everywhere. \qed

The trick, then, is to specify $F$ so that $A(F)$ is a set of OT maps. Recalling that each $A_{a,b} \in A(F)$ is of the form $f_b^{-1} \circ f_a$, we see that if $T_c$ forms a group (where the group operation is function composition),\footnote{The relevant group properties are that $T_c$ is closed under composition and has unique inverse elements.} then setting $F = T_c$ implies that $A_{a,b} = f_b^{-1} \circ f_a \in T_c$ and Theorem 5.1 holds.

**Proposition 5.2.** If $T_c$ forms a group under composition then the model $M(F = T_c, \{P_z^e\}_{e \in E}, \lambda_z)$ is strongly identifiable for any $|E| \geq 1$. 

PROOF. \( A(F) = A(T_c) \) consists of compositions of elements of \( T_c \), hence \( A(F) \subseteq T_c \). By Theorem 5.1, this model is strongly identifiable.

This is not the only way to specify a strongly identifiable model via transport indeterminacies, but it may be the most straightforward. We give two examples based on known transport maps to illustrate. The first shows that with an appropriate group of transport maps \( T \), we do not even need optimality, as long as the only element of \( T \) that fixes \( P_z \) is the identity. The second highlights a difficulty with model specification using Brenier maps.

5.1.1. Knöthe–Rosenblatt (KR) transports. Triangular monotone increasing (TMI) maps are of growing interest in generative modelling [21, 31, 17, 42, 16]. More generally, many normalizing flow [30] models have triangular, even monotonic layers, but due to alternating between lower and upper-triangular (see [6, 7, 37]) the final generator may fail to be triangular monotone. The KR transport between two fully supported probability measures \( P_a, P_b \) has an explicit construction as a TMI map, in terms of one-dimensional conditional CDF transforms. See Appendix C for details.

Though it is not known to be an optimal transport map itself, it is the limit of optimal transport maps for a sequence of appropriately weighted quadratic losses [34, Ch. 2.4]. For our purposes, it is more important that the KR transport is the unique (up to almost everywhere equivalence) TMI map that transports between \( P_a \) and \( P_b \), and that the class of such maps are closed under composition and inversion. For more details on its construction and properties, as well as the proof of the following results, see Appendix C.

**Theorem 5.3.** Let \( Z = X = \mathbb{R}^d \), and \( \mathcal{P}^e_z = \{ P^e_z \} \), where for each \( e \in E \), \( P^e_z \ll \lambda_z \) is any fixed probability distribution on \( \mathbb{R}^d \) with strictly positive density. If \( \mathcal{F} \) consists entirely of triangular monotone increasing maps, then \( M(\mathcal{F}, \{ P^e_z \}_{e \in E}, \lambda_z) \) is strongly identifiable for any \( |E| \geq 1 \).

Such a generator class also provides identifiability in the ICA sense—we thus believe the following result may also be of independent interest to the ICA community.

**Proposition 5.4.** Let \( Z = X = \mathbb{R}^d \). The ICA model with \( M(\mathcal{F}, \mathcal{P}_z, \lambda_z) \) with \( \mathcal{F} \) (mixing functions) consisting entirely of triangular monotone increasing maps and \( \mathcal{P}_z \) fully supported
distributions with independent components is identifiable up to invertible, component-wise transformations.

5.1.2. Brenier map indeterminacies. Brenier maps have appeared recently in a number of machine learning contexts \[2, 11, 40\]. They are the unique solutions to the OT problem with \(c(z_1, z_2) = ||z_1 - z_2||^2\), and are characterized by the property that a Brenier map \(A\) is the gradient of a convex function, \(A = \nabla \phi\), for convex \(\phi : \mathbb{R}^d \to \mathbb{R}\). The set of Brenier maps is not closed under composition, and therefore poses some difficulties to specifying \(F\). To our knowledge, the only way to achieve \(A(F) \subseteq \mathcal{T}_{||z_1 - z_2||^2}\) is for every \(f_a, f_b \in F\) to be cyclically co-monotone, a property deduced recently in \[38\]. That is, \(f_a, f_b\) must satisfy, for each \(m \in \mathbb{N}\) and each sequence \(z_1, z_2, \ldots, z_{m+1} = z_1\),

\[
\sum_{i=1}^{m} \langle f_b(z_i), f_a(z_{i+1}) - f_a(z_i) \rangle \geq 0.
\]

We do not know of any general (and flexible) function classes that satisfy this property.

6. Discrete Observations. In this section, we briefly discuss models with discrete observations, e.g., Bernoulli with probability parameter given by \(f(z)\), or Poisson with mean parameter \(f(z)\) (such models were briefly discussed in iVAE \[19\], as well as in follow-up work such as the pi-VAE \[45\]). In short, the framework developed in this paper rests on bijective generators which enable the recovery of unique latent codes for each observed value. As noted in a correction in \[19\], this task seems fundamentally impossible for example when the latent space is uncountable and the outcome is discrete, due to the lack of an bijective map between spaces of different cardinality. However, generative models do not typically send a latent variable to the outcome, but rather to a parameter value of a conditional distribution. This allows us to reformulate the assumptions required for our theory, although as we will see shortly, most discrete outcome models do not satisfy these assumptions.

Formally, suppose \(X\) is either finite or countable. Let \(X\) be a random variable on \(X\) and denote by \(P_x := P(X = x) : X \to [0, 1]\) the probability mass function, which satisfies \(\sum_{x \in X} P_x(x) = 1\). Two random variables \(X_a, X_b\) are said to be equal in distribution if and only if their respective PMFs satisfy \(P_{x,a}(x) = P_{x,b}(x)\) for all \(x \in X\).

The observation model is then described by a conditional PMF \(P(X = x \mid z)\). We assume this model has a topological parameter space \(\Theta\) and also pair it with the Borel \(\sigma\)-algebra, e.g.,
18

\[ \Theta = [0, 1]^n \] for an \( n \)-dimensional Bernoulli. Let \( f : \mathbb{Z} \to \Theta \) be an injective generator (note this implies \( \Theta \) has cardinality at least that of \( \mathbb{Z} \)). Then the generative model is as follows:

\begin{equation}
Z \sim P_z, \quad P(X = x | z) = g_x(f(z)),
\end{equation}

where \( g_x(\theta) \) is the PMF of the observation model with parameter \( \theta \) at \( x \).

Recall Assumption 1. We now introduce its discrete analogue, which would be required for the theory developed in this paper. First, note that the marginal PMF on \( X \) is given as follows:

\begin{equation}
P_x(x) = \int_{\mathbb{Z}} g_x(f(z))P_z(dz) = \int_{\Theta} g_x(\theta)P_z(f^{-1}(d\theta)) = \mathbb{E}_\theta[g_x(\theta)],
\end{equation}

where as a random variable, \( \theta = f(Z) \). The assumption is then as follows:

**Assumption 3** (Discrete analogue to Assumption 1). Assume that \( \mathbb{E}_{\theta_a}[g_x(\theta_a)] = \mathbb{E}_{\theta_b}[g_x(\theta_b)] \) for each \( x \in \mathbb{X} \) if and only if \( \theta_a \not \equiv \theta_b \).

In other words, the distribution of \( \theta = f(Z) \) must be characterized by the moments \( \mathbb{E}[g_x(\theta_a)] \), for each \( x \in \mathbb{X} \). Indeed, for observational equivalence to imply anything about the latent spaces, such an assumption would be needed. However, it appears that this assumption is rarely satisfied for any reasonable models. For example, the Bernoulli observation model with \( P(X = 1 | z) = g_1(\theta) = \theta, \Theta = [0, 1] \), requires that the distribution of \( \theta \) be characterized by just its first moment, \( \mathbb{E}[\theta] \). Of course, this is highly unlikely unless very strict restrictions are placed on \( f \) and \( P_z \).

At the core of the issue remains the cardinality mismatch between \( \mathbb{Z} \) and \( \mathbb{X} \). One necessary condition to show that \( \theta_a \not \equiv \theta_b \) is that \( \mathbb{E}[g(\theta_a)] = \mathbb{E}[g(\theta_b)] \) for all bounded continuous \( g : \Theta \to \mathbb{R} \) (test functions). For \( \Theta \) uncountable, there are clearly uncountably many test functions, while in our discrete assumption above, there are countably many test functions at best. Though we do not make this notion precise here, we believe this makes the discrete assumption above unlikely to be satisfied, and hence identifiability, at least under our framework (which we believe to be reasonably general), is highly unlikely for discrete outcomes with uncountable latent spaces.

**7. Conclusion.** We have developed a general formal framework for analyzing the sources of unidentifiability in a broad class of latent variable models. The framework brings
seemingly disparate approaches to the problem together. Importantly, it also makes the sources of indeterminacy visible, enabling more straightforward reasoning about them when designing models. That visibility was crucial to our novel strong identifiability results, particularly to the transport-based models in Section 5. Those models are far from exhaustive, and we believe that our framework can be useful in developing novel strongly identifiable latent variable models.

REFERENCES

[1] Ahuja, K., Hartford, J. and Bengio, Y. (2022). Properties from Mechanisms: An Equivariance Perspective on Identifiable Representation Learning. In ICLR 2022.
[2] Amos, B., Xu, L. and Kolter, J. (2017). Input Convex Neural Networks. In ICML 2017.
[3] Arjovsky, M., Bottou, L., Gulrajani, I. and Lopez-Paz, D. (2019). Invariant Risk Minimization. arXiv preprint arXiv:1907.02893.
[4] Bühlmann, P. (2020). Invariance, Causality and Robustness. Statistical Science 35 404 – 426.
[5] Comon, P. (1994). Independent component analysis, A new concept? Signal Processing 36 287-314.
[6] Dinh, L., Krueger, D. and Bengio, Y. (2015). NICE: Non-linear Independent Components Estimation. In Workshop at ICLR 2015.
[7] Dinh, L., Sohl-Dickstein, J. and Bengio, S. (2017). Density Estimation using Real NVP. In ICLR 2017.
[8] Gresele, L., Kügelgen, J. V., Stimper, V., Schölkopf, B. and Besserve, M. (2021). Independent Mechanism analysis, a New Concept? In NeurIPS 2021.
[9] Gresele, L., Rubenstein, P. K., Mehrjou, A., Locatello, F. and Schölkopf, B. (2019). The Incomplete Rosetta Stone Problem: Identifiability Results for Multi-View Nonlinear ICA. In UAI 2019.
[10] Halva, H., Corff, S. L., Lehéricy, L., So, J., Zhu, Y., Gassiat, E. and Hyvärinen, A. (2021). Disentangling Identifiable Features from Noisy Data with Structured Nonlinear ICA. In NeurIPS 2021.
[11] Huang, C.-W., Chen, R. T. Q., Tsirigotis, C. and Courville, A. (2021). Convex Potential Flows: Universal Probability Distributions with Optimal Transport and Convex Optimization. In ICLR 2021.
[12] Hyvärinen, A. and Morioka, H. (2016). Unsupervised Feature Extraction by Time-Contrastive Learning and Nonlinear ICA. In NeurIPS 2016.
[13] Hyvärinen, A. and Morioka, H. (2017). Nonlinear ICA of Temporally Dependent Stationary Sources. In AISTATS 2017.
[14] Hyvärinen, A. and Paajanen, P. (1999). Nonlinear Independent Component Analysis: Existence and Uniqueness Results. Neural Networks 12 429–439.
[15] Hyvärinen, A., Sasaki, H. and Turner, R. E. (2018). Nonlinear ICA Using Auxiliary Variables and Generalized Contrastive Learning. In AISTATS 2019 859–868.
[16] Irons, N. J., Scetbon, M., Pal, S. and Harchaoui, Z. (2021). Triangular Flows for Generative Modeling: Statistical Consistency, Smoothness Classes, and Fast Rates. arXiv preprint arXiv:2112.15595.
[17] Jaini, P., Selby, K. A. and Yu, Y. (2019). Sum-of-Squares Polynomial Flow. In ICML 2019.
[18] Kechris, A. S. (1995). Classical Descriptive Set Theory. Springer.
[19] Khemakhem, I., Kingma, D. P., Monti, R. P. and Hyvärinen, A. (2020). Variational Autoencoders and Nonlinear ICA: A Unifying Framework. In AISTATS 2020.
[20] Khemakhem, I., Monti, R. P., Kingma, D. P. and Hyvärinen, A. (2020). ICE-BeeM: Identifiable Conditional Energy-Based Deep Models Based on Nonlinear ICA. In NeurIPS 2020.
[21] Kingma, D. P., Salimans, T., Jozefowicz, R., Chen, X., Sutskever, I. and Welling, M. (2016). Improved Variational Inference with Inverse Autoregressive Flow. In NeurIPS 2016.
[22] Klindt, D., Schott, L., Sharma, Y., Ustyuzhaninov, I., Brendel, W., Bethge, M. and Palton, D. M. (2021). Towards Nonlinear Disentanglement in Natural Data with Temporal Sparse Decoding. In ICLR 2021.
[23] Lawley, D. N. and Maxwell, A. E. (1962). Factor Analysis as a Statistical Method. Journal of the Royal Statistical Society, Series D (The Statistician) 12 209–229.
[24] Locatello, F., Bauer, S., Lucic, M., Ratsch, G., Gelly, S., Schölkopf, B. and Bachem, O. (2019). Challenging Common Assumptions in the Unsupervised Learning of Disentangled Representations. In ICML 2019 4114–4124.
[25] Locatello, F., Poole, B., Ratsch, G., Schölkopf, B., Bachem, O. and Tshannen, M. (2020). Weakly-Supervised Disentanglement Without Compromises. In ICML 2020.
[26] Lu, C., Wu, Y., Hernández-Lobato, J. M. and Schölkopf, B. (2022). Invariant Causal Representation Learning for Out-of-Distribution Generalization. In ICLR 2022.
[27] Maritz, J. S. and Lwin, T. (1989). Empirical Bayes Methods. CRC Press.
[28] Mita, G., Filippone, M. and Michardi, P. (2021). An Identifiable Double VAE For Disentangled Representations. In ICML 2021.
[29] Moran, G. E., Sridhar, D., Wang, Y. and Blei, D. M. (2021). Identifiable Variational Autoencoders via Sparse Decoding. arXiv preprint arXiv:2110.10804.
[30] Papamakarios, G., Nalisnick, E., Rezende, D. J., Mohamed, S. and Lakshminarayanan, B. (2021). Normalizing Flows for Probabilistic Modeling and Inference. Journal of Machine Learning Research 22 1-64.
[31] Papamakarios, G., Pavlakou, T. and Murray, I. (2017). Masked Autoregressive Flow for Density Estimation. In NeurIPS 2017.
[32] Peters, J., Bühlmann, P. and Meinshausen, N. (2016). Causal inference by using invariant prediction: identification and confidence intervals. Journal of the Royal Statistical Society: Series B (Statistical Methodology) 78 947-1012.
[33] Rudin, W. (1987). Real and Complex Analysis. McGraw–Hill.
[34] Santambrogio, F. (2015). Optimal Transport for Applied Mathematicians. Birkhäuser Cham.
[35] Schilling, R. L. (2005). *Measures, Integrals and Martingales*. Cambridge University Press.

[36] Scholkopf, B., Locatello, F., Bauer, S., Ke, N. R., Kalchbrenner, N., Goyal, A. and Ben-gio, Y. (2021). Toward causal representation learning. *Proceedings of the IEEE* **109** 612–634.

[37] Sorrenson, P., Rother, C. and Köthe, U. (2020). Disentanglement by Nonlinear ICA with General Incompressible-flow Networks (GIN). In *ICLR 2020*.

[38] Torous, W., Gunsilius, F. and Rigollet, P. (2021). An Optimal Transport Approach to Causal Inference. *arXiv preprint arXiv:2108.05858*.

[39] Van der Vaart, A. (1998). *Asymptotic Statistics*. Cambridge University Press.

[40] Wang, Y., Blei, D. and Cunningham, J. P. (2021). Posterior Collapse and Latent Variable Non-identifiability. In *NeurIPS 2021*.

[41] Wang, Y. and Jordan, M. I. (2021). Desiderata for Representation Learning: A Causal Perspective. *arXiv preprint arXiv:2109.03795*.

[42] Wehkelkel, A. and Louppe, G. (2019). Unconstrained Monotonic Neural Networks. In *NeurIPS 2019*.

[43] Willetts, M. and Paige, B. (2021). I Don’t Need u: Identifiable Non-Linear ICA without Side Information. *arXiv preprint arXiv:2106.05238*.

[44] Yang, M., Liu, F., Chen, Z., Shen, X., Hao, J. and Wang, J. (2021). CausalVAE: Disentangled Representation Learning via Neural Structural Causal Models. In *CVPR 2021*.

[45] Zhou, D. and Wei, X.-X. (2020). Learning identifiable and interpretable latent models of high-dimensional neural activity using pi-VAE. In *NeurIPS 2020*. 
APPENDIX A: DEFINITIONS

In this section, we review some relevant measure theoretic notions. Let $E$ be a topological space. A collection $\mathcal{E}$ of subsets of $E$ is called a $\sigma$-algebra on $E$ if it is closed under complements and countable unions:

\begin{equation}
B \in \mathcal{E} \implies E \setminus B \in \mathcal{E}, \quad B_1, B_2, \cdots \in \mathcal{E} \implies \bigcup_n A_n \in \mathcal{E}.
\end{equation}

A $\sigma$-algebra always contains the empty set and $E$ itself. The pair $(E, \mathcal{E})$ defines a measurable space. The elements of $\mathcal{E}$ in this context are called measurable sets. The $\sigma$-algebra generated by a collection of subsets $\mathcal{E}'$, denoted $\sigma(\mathcal{E}')$ is the smallest $\sigma$-algebra that contains $\mathcal{E}'$.

In our setting, we will almost always work with the Borel $\sigma$-algebra generated by the collection of open sets of $E$, denoted $\mathcal{B}(E)$. An element $B \in \mathcal{B}(E)$ is then said to be a Borel set.

Let $(E, \mathcal{E})$, $(F, \mathcal{F})$ be two measurable spaces, and $f : E \to F$ a mapping between them. The preimage of $B \subset F$ is denoted

\begin{equation}
f^{-1}(B) = \{ x \in E \mid f(x) \in B \}.
\end{equation}

A mapping $f$ is said to be $(\mathcal{E}, \mathcal{F})$-measurable if $f^{-1}(B) \in \mathcal{E}$ for each $B \in \mathcal{F}$. It is also called a Borel function if it is $(\mathcal{B}(E), \mathcal{B}(F))$-measurable. If $(E, \mathcal{E}) = (F, \mathcal{F})$, we will refer to $f$ as simply $\mathcal{E}$-measurable.

A measure on $(E, \mathcal{E})$ is a mapping $\mu : \mathcal{E} \to [0, \infty]$ such that:

\begin{equation}
\mu(\emptyset) = 0, \quad \mu(\bigcup_n A_n) = \sum_n \mu(A_n), \quad (A_n) \text{ a disjoint sequence in } \mathcal{E}.
\end{equation}

$\mu$ is a probability measure if further $\mu(E) = 1$. The triplet $(E, \mathcal{E}, \mu)$ is known as a measure space, and, if $\mu$ is a probability measure, as a probability space. Two measures $\mu$ and $\nu$ on the same measurable space are equal whenever

\begin{equation}
\mu(B) = \nu(B), \quad \text{for all } B \in \mathcal{E}.
\end{equation}

A property $P$ that is stated for $x \in E$ is said to hold $\mu$-almost everywhere if there exists a measurable set $N$ with $\mu(N) = 0$ such that $P$ holds for all $z \in E \setminus N$.

A random variable $X$ on $(E, \mathcal{E})$ are associated to a probability measure $\mu$ called its distribution, defined as

\begin{equation}
P(X \in B) = \mu(B), \quad \text{for all } B \in \mathcal{E}.
\end{equation}
Random variables $X$, $Y$ defined on the same measurable space with distributions $\mu$, $\nu$ are said to be equal in distribution if $\mu = \nu$ as probability measures, denoted $X \overset{d}{=} Y$. Any $(\mathcal{E}, \mathcal{F})$-measurable function $f : E \to F$ applied to $X$, denoted $f(X)$, defines a random variable on $(F, \mathcal{F})$ with distribution $\mu \circ f^{-1}$, where $f^{-1}$ denotes the preimage of $f$ as a set function $\mathcal{F} \to \mathcal{E}$.

APPENDIX B: PROOFS

B.1. Proofs for Section 3. We first recall Assumption 2 on the class of generators $\mathcal{F}$:

**Assumption 2.** Assume that any $f \in \mathcal{F}$ is injective, and has the same image: for any $f_a, f_b \in \mathcal{F}$, $f_a(Z) = f_b(Z) := \mathcal{F}(Z) \subseteq X$.

Further note that we assumed $f$ to be $(\mathcal{B}(\mathcal{Z}), \mathcal{B}(\mathcal{X}))$-measurable, i.e., it is Borel. We have a preliminary fact about injective Borel functions.

**Lemma B.1** (Corollary 15.2, [18]). For $f$ Borel and injective, $f(B)$ (the image) is a Borel set for all Borel sets $B \in \mathcal{B}(\mathcal{Z})$.

Recall that $A_{a,b} : \mathcal{Z} \to \mathcal{Z}$ is given by $A_{a,b}(z) = f_b^{-1}(f_a(z))$, where $f_a, f_b \in \mathcal{F}$. We show that this map is a Borel automorphism.

**Lemma B.2.** $A_{a,b}$ is invertible, and both $A_{a,b}$ and $A_{a,b}^{-1}$ are $\mathcal{B}(\mathcal{Z})$-measurable.

**Proof.** $A_{a,b}$ is clearly invertible, being the composition of invertible functions. The pre-image of $A_{a,b}$ is $f_a^{-1} \circ f_b$, since $\mathcal{F}$ is a family of injective functions. By definition of measurability, it suffices to show that $f_a^{-1}(f_b(B)) \subseteq \mathcal{Z}$ is still Borel for any Borel set $B \in \mathcal{B}(\mathcal{Z})$. By Lemma B.1, $f_b(B) \subseteq \mathcal{X}$ is Borel. Then, by measurability of $f_a$, it follows that $f_a^{-1}(f_b(B))$ is Borel and hence $A_{a,b}$ is measurable.

The pushforward $\sigma$-algebra of the bijection $f : \mathcal{Z} \to \mathcal{F}(\mathcal{Z})$ is the following collection of subsets of $\mathcal{F}(\mathcal{Z})$:

$$\sigma(f) = \{ B \subseteq \mathcal{F}(\mathcal{Z}); f^{-1}(B) \in \mathcal{B}(\mathcal{Z}) \}$$

(6) It is easily shown that $\sigma(f)$ is a $\sigma$-algebra on $\mathcal{F}(\mathcal{Z})$, and that $f$ is $(\mathcal{B}(\mathcal{Z}), \mathcal{F}(\mathcal{Z}))$-measurable.
Lemma B.3. Suppose \( f \in \mathcal{F} \). Then, \( \sigma(f) \) contains only Borel sets. In other words, \( \sigma(f) \subset \mathcal{B}(\mathcal{X}) \).

Proof. Let \( C \in \sigma(f) \). By definition, \( f^{-1}(C) \) is Borel. Since \( f \) is injective, we have \( f(f^{-1}(C)) = C \). By Lemma B.1, \( C \) must be Borel.

Further, all generators in \( \mathcal{F} \) induce the same pushforward \( \sigma \)-algebra.

Lemma B.4. For \( f_a, f_b \) in \( \mathcal{F} \), \( \sigma(f_a) = \sigma(f_b) \).

Proof. To see that \( \sigma(f_a) \subset \sigma(f_b) \), suppose \( C \in \sigma(f_a) \). By Lemma B.3, \( C \) is Borel, which means that \( f_b^{-1}(C) \) is Borel by measurability. Hence, \( C \in \sigma(f_b) \). We have \( \sigma(f_b) \subset \sigma(f_a) \) by the exact same argument, which implies that \( \sigma(f_a) = \sigma(f_b) \).

We denote this shared \( \sigma \)-algebra by \( \sigma(\mathcal{F}) \). The reason we work with \( \sigma(\mathcal{F}) \) is to construct the measurable space \( (\mathcal{F}(\mathcal{Z}), \sigma(\mathcal{F})) \). Note the following facts about \( (\mathcal{F}(\mathcal{Z}), \sigma(\mathcal{F})) \):

- For any \( f \in \mathcal{F} \), \( f : \mathcal{Z} \to \mathcal{F}(\mathcal{Z}) \) is bijective, and \( f^{-1} : \mathcal{F}(\mathcal{Z}) \to \mathcal{Z} \) is well defined.
- For any \( f \in \mathcal{F} \) and a Borel set \( B \in \mathcal{B}(\mathcal{Z}) \), its image \( f(B) \subset \mathcal{F}(\mathcal{Z}) \) is also the pre-image of \( f^{-1} \)—that is, \( (f^{-1})^{-1}(B) = f(B) \).
- Since \( \sigma(\mathcal{F}) \subset \mathcal{B}(\mathcal{X}) \), if any measures are equal on \( \mathcal{B}(\mathcal{X}) \), then they are also equal on \( \sigma(\mathcal{F}) \).

We now restate and prove our main Lemma about the indeterminacy map:

Lemma 3.1. Let \( \theta_a = (P_{z,a}, f_a) \) and \( \theta_b = (P_{z,b}, f_b) \) be two parametrizations of a generative model with resulting marginal distributions \( P_{\theta_a} \) and \( P_{\theta_b} \). Then, \( P_{\theta_a} = P_{\theta_b} \) if and only if \( P_{z,a} = P_{z,b} \circ A_{a,b}^{-1} \) and \( P_{z,a} = P_{z,b} \circ A_{a,b} \), where \( A_{a,b} \) is the indeterminacy map (5).

Proof. \( \implies \) : Recall that \( A_{a,b} \) and \( A_{a,b}^{-1} \) are measurable. By Assumption 1 in the main text, \( P_{\theta_a} = P_{\theta_b} \) implies that \( P_{z,a} \circ f_a^{-1} = P_{z,b} \circ f_b^{-1} \) on \( \mathcal{B}(\mathcal{X}) \), which implies equality also for \( \sigma(\mathcal{F}) \). Let \( B \in \mathcal{B}(\mathcal{Z}) \). Then,

\[
P_{z,a}(A_{a,b}^{-1}(B)) = P_{z,a}(f_a^{-1}(f_b(B))) = P_{z,b}(f_b^{-1}(f_b(B))) = P_{z,b}(B),
\]

where the first equality is by definition (working on \( \sigma(\mathcal{F}) \)), the second equality is due to \( P_{z,a} \circ f_a^{-1} = P_{z,b} \circ f_b^{-1} \), and the third equality is due to injectivity. Since \( B \) was arbitrary, this shows that \( P_{z,a} \circ A_{a,b}^{-1} = P_{z,b} \). To see that \( P_{z,a} = P_{z,b} \circ A_{a,b} \), simply swap the roles of the indices \( a \) and \( b \)
Without loss of generality, suppose that \( P_z, b \neq P_z, a \circ A_{a, b}^{-1} \) (the same argument works for \( P_z, a \neq P_z, b \circ A_{a, b} \)). Note that by Assumption 1, it is equivalent to show that \( P_z, a \circ f_a^{-1} \neq P_z, b \circ f_b^{-1} \). That is, we aim to find some \( B \in \mathcal{B}(\mathbb{X}) \) such that

\[
P_z, a (f_a^{-1}(B)) \neq P_z, b (f_b^{-1}(B)).
\]

To construct such a \( B \), let \( B^* \in \mathcal{B}(\mathbb{Z}) \). We have by hypothesis that

\[
P_z, a (B^*) \neq P_z, a (A_{a, b}^{-1}(B^*)) = P_z, a (f_a^{-1}(f_b(B^*)�).
\]

We have \( f_b(B^*) \subset \mathbb{X} \), which is a Borel set by Lemma B.1. Then,

\[
P_z, a (f_a^{-1}(f_b(B^*)) \neq P_z, a (B^*) = P_z, a (f_a^{-1}(f_a(B^*))�,
\]

and hence taking \( B = f_b(B^*) \) shows that \( P_z, a \circ f_a^{-1} \neq P_z, b \circ f_b^{-1} \). \( \square \)

Finally, we prove Theorem 3.2.

**Theorem 3.2.** The generative model \( \mathcal{M}(\mathcal{F}, \mathcal{P}_{z, \mu_{z}}) \) is identifiable up to \( \mathcal{A}(\mathcal{M}) = \mathcal{A}(\mathcal{F}) \cap \mathcal{A}(\mathcal{P}_{z}) \). In particular, \( \mathcal{M}(\mathcal{F}, \mathcal{P}_{z, \mu_{z}}) \) is strongly identifiable if and only if \( \mathcal{A}(\mathcal{F}) \cap \mathcal{A}(\mathcal{P}_{z}) = \widetilde{id}_{z} \).

**Proof.** Recall that, for the generative model to be identifiable up to a set of measurable functions \( \mathcal{A}(\mathcal{M}) \) is to say that, for all \((f_a, P_z, a), (f_b, P_z, b) \in \mathcal{F} \times \mathcal{P}_z \) such that \( P_{\theta_a} = P_{\theta_b} \), we have \( A = f_b^{-1} \circ f_a \in \mathcal{A}(\mathcal{M}) \).

We first show that for any parameter spaces \( \mathcal{F} \) and \( \mathcal{P}_z \), we have that \( \mathcal{A}(\mathcal{M}) \subseteq \mathcal{A}(\mathcal{F}) \cap \mathcal{A}(\mathcal{P}_z) \). Suppose \( A \in \mathcal{A}(\mathcal{M}) \). That is, \( A = f_b^{-1} \circ f_a \) such that there exist \( P_{z, a}, P_{z, b} \) such that the parametrizations \( \theta_a = (f_a, P_z, a), \theta_b = (f_b, P_z, b) \) have \( P_{\theta_a} = P_{\theta_b} \). By definition of \( A \), we have \( A \in \mathcal{A}(\mathcal{F}) \). By Lemma 3.1, we must have that \( A \in \mathcal{A}(\mathcal{P}_z) \) also.

We now show that \( \mathcal{A}(\mathcal{F}) \cap \mathcal{A}(\mathcal{P}_z) \subseteq \mathcal{A}(\mathcal{M}) \). Suppose \( A \in \mathcal{A}(\mathcal{F}) \cap \mathcal{A}(\mathcal{P}_z) \). We can write \( A = f_b^{-1} \circ f_a \) for some \( f_a, f_b \in \mathcal{F} \). Furthermore, there exist \( P_{z, a} \) and \( P_{z, b} \) such that \( P_{z, b} = P_{z, a} \circ A^{-1} \) and \( P_{z, a} = P_{z, b} \circ A \). By Lemma 3.1, \( \theta_a = (f_a, P_z, a), \theta_b = (f_b, P_z, b) \) is such that \( P_{\theta_a} = P_{\theta_b} \), and hence \( A \in \mathcal{A}(\mathcal{M}) \). \( \square \)
B.2. Proofs for Section 4. We first prove Corollary 4.1.

**COROLLARY 4.1.** The generative model \( M(\mathcal{F}, \{P^e_z\}_{e \in E}, \mu_z) \) is identifiable up to
\[
A(\mathcal{F}) \cap (\cap_{e \in E} A(P^e_z)) .
\]

**PROOF.** We can view identifiability of the multiple environments model as simultaneous identifiability for sub-models, each corresponding to an environment. That is, Theorem 3.2 applies in each environment. Hence, for any pre-composition indeterminacy \( A \), we have
\[
A \in \bigcap_e (A(\mathcal{F}) \cap A(P^e_z)) = A(\mathcal{F}) \cap (\cap_{e \in E} A(P^e_z)) .
\]

\( \Box \)

We now prove identifiability for the equivariant stochastic mechanisms model.

**PROPOSITION 4.2.** The model described by (9) is identifiable up to \( A \in A(M) \) satisfying
\[
A(m_a(Z, U)) \overset{d}{=} m_b(A(Z), U),
\]
for any \( m_a, m_b \in M \), \( U \sim U[0, 1] \) and any random variable \( Z \) independent of \( U \).

**PROOF.** We can analyze this model in our framework using just two time-points, \( t = 1, 2 \). We work on an augmented latent space \( \tilde{Z} = Z \times [0, 1] \) and treat the random variables \( U_t \) as additional latent variables. For a generator \( f : Z \to X \), we extend \( \tilde{f} : \tilde{Z} \to X \times [0, 1] \), \( \tilde{f}(z, u) = (f(z), u) \). The identity extension ensures that \( \tilde{f} \) is still injective, and is unique to \( f \). Now suppose \( f_a \) and \( f_b \) are such that the distribution of \( X_1 \) and \( X_2 | X_1 \) match. Note the marginal and conditional uniquely determine the joint, and hence we simply assume that the joint and hence marginal distributions of \( X_1 \) and \( X_2 \) match.

Let the joint distribution of \( Z_1 \) and \( U \) be denoted \( \pi_{Z_1,U} \). Since they are independent, we have that \( \pi_{Z_1,U} = P_1 \otimes U[0, 1] \).\(^5\) We also extend the mechanism \( m \) as \( \tilde{m}(z, u) = (m(z, u), u) \), implying that \( \tilde{m}^{-1}(B_z \times B_u) = m^{-1}(B_z) \times B_u \). Since \( Z_2 = m(Z_1, U_1) \), this then implies that \( P_2 = \pi_{Z_1,U} \circ \tilde{m}^{-1} = (P_1 \circ m^{-1}) \otimes (U[0, 1]) \) (note the standard \( m \) in the right-hand-side). The same applies to an extended indeterminacy map, i.e., \( P_2 \circ \tilde{A}_{a,b} = (P_1 \circ \tilde{A}^{-1}_{a,b}) \otimes (U[0, 1]) \).

\(^5\)This means that for a Borel product \( B_z \times B_u \), where \( B_z, B_u \) are Borel sets in their respective domains, we have \( \pi_{X_1,U}(B_z \times B_u) = (P_1(B_z))(U[0, 1][B_u]) \).
We now apply Lemma 3.1 to \( t = 1 \), where \( Z_1 \) has fixed distribution \( P_1 \) (i.e., it is a singleton), and to \( t = 2 \), where the latent distribution may vary with the mechanism \( m_a \) or \( m_b \), denoted \( P_{2,a}, P_{2,b} \). As a result, we obtain

\[
P_1 = P_1 \circ A_{a,b}^{-1}, \quad P_{2,b} = P_{2,a} \circ \tilde{A}_{a,b}^{-1}.
\]

Applying these identities simultaneously to \( P_{2,b} \) gives

\[
P_{2,b} = (P_1 \circ m_b^{-1}) \otimes (U[0,1]) = (P_1 \circ A_{a,b}^{-1} \circ m_b^{-1}) \otimes (U[0,1])
\]

\[
P_{2,b} = P_{2,a} \circ \tilde{A}_{a,b}^{-1} = (P_1 \circ m_a^{-1} \circ A_{a,b}^{-1}) \otimes (U[0,1]),
\]

which by the properties of a product measure, means that

\[
(P_1 \circ A_{a,b}^{-1} \circ m_b^{-1}) = (P_1 \circ m_a^{-1} \circ A_{a,b}^{-1}).
\]

Writing the above in terms of their random variables, we have \( m_b(A_{a,b}(Z), U) \) \( \overset{d}{=} \) \( A_{a,b}(m_a(Z, U)) \) for \( Z \) with any fixed distribution \( P_1 \) independent of \( U \).

We now work towards proving identifiability of the iVAE, and our proposed strongly identifiable extension. First we need some preliminaries. For the rest of this section, recall that \( Z = \mathbb{R}^d \). Let \( \lambda_z \) denote the d-dimensional Lebesgue measure. Recall that a probability measure \( P \) is said to be absolutely continuous with respect to \( \lambda_z \), denoted \( P \ll \lambda_z \), if for any Borel set \( B \),

\[
\lambda_z(B) = 0 \implies P(B) = 0.
\]

If \( P \ll \lambda_z \) and \( \lambda_z \ll P \), we say that \( P \) is equivalent to \( \lambda_z \).

For a property that holds \( \lambda_z \)-almost everywhere (equivalently, \( P \)-almost everywhere for an equivalent measure \( P \)), we simply refer to it as holding almost everywhere (a.e.). Recall that for a measure \( P \ll \lambda_z \), there exists a density (with respect to \( \lambda_z \)) function \( p : \mathbb{R}^d \to [0, \infty) \) that is unique a.e.. We have the following fact:

**Lemma B.5 ([35], Problem 19.5).** A probability measure \( P \) has a strictly positive density a.e. if and only if it is equivalent to \( \lambda_z \).

Now, we may state an intermediate result. Recall that an invertible bi-measurable function \( A : \mathbb{R}^d \to \mathbb{R}^d \) is called a \( (P_{z,a}, P_{z,b}) \)-measure isomorphism if \( P_{z,a} = P_{z,b} \circ A \) and \( P_{z,b} = P_{z,a} \circ A^{-1} \).
Lemma B.6. Suppose probability measures $P_{z,a}, P_{z,b}$ admits strictly positive densities $p_a, p_b$. Suppose $A$ is a ($P_{z,a}$, $P_{z,b}$)-measure isomorphism. Then,

$$p_b(A(x))k_A(x) = p_a(x) \quad \text{a.e.},$$

where $k_A$ depends only on $A$ and is strictly positive a.e..

Proof. Since $A$ is a ($P_{z,a}$, $P_{z,b}$)-measure isomorphism and $P_{z,a}, P_{z,b}$ are equivalent to $\lambda_z$, we have that for a Borel set $B$,

$$\lambda_z(B) = 0 \iff P_{z,a}(B) = 0 \iff P_{z,b}(A(B)) = 0 \iff \lambda_z(A(B)) = 0,$$

where the first and third equivalences are because $P_{z,a}$ and $P_{z,b}$ are equivalent to $\lambda_z$. This shows that $\lambda_z \circ A$ is equivalent to $\lambda_z$, and hence it has an a.e.-strictly positive density $k_A$. Then, by the definition of the density (Radon-Nikodym derivative), we have for a Borel set $B$,

$$P_{z,a}(B) = P_{z,b}(A(B))$$

$$\iff \int_B p_a(x) \lambda_z(dx) = \int_{A(B)} p_b(x) \lambda_z(dx) = \int_{A(B)} p_b(A(x)) \lambda_z(A(dx)),$$

where the last equality is by the standard change of variables formula, noting that $B = A^{-1}(A(B))$ since $A$ is invertible. Now, we have that

$$\int_B p_a(x) \lambda_z(dx) = \int_B p_b(A(x))k_A(x) \lambda_z(dx),$$

by invoking the definition of the density again. Since the above holds for any $B$, we have

$$p_b(A(x))k_A(x) = p_a(x) \quad \text{a.e.},$$

where $k_A(x)$ is strictly positive a.e.. \qed

Corollary B.7. Suppose four probability measures $P_{1,a}, P_{2,a}, P_{1,b}, P_{2,b}$ have strictly positive densities $p_{1,a}, p_{2,a}, p_{1,b}, p_{2,b}$. For $A$ both a ($P_{1,a}, P_{1,b}$)-measure isomorphism and a ($P_{2,a}, P_{2,b}$)-measure isomorphism, we have

$$\frac{p_{1,a}(x)}{p_{2,a}} = \frac{p_{1,b}(A(x))}{p_{2,b}} \quad \text{a.e.}.$$

Proof. This follows immediately from Lemma B.6 from the fact that $k_A$ is strictly positive a.e. and depends only on $A$. \qed
To prove identifiability of iVAE, we first recall some notation for an exponential family distribution. For a probability distribution varying by a variable $u$ with density

$$p(z|u) = m(z) \exp(\eta(u)^\top T(z) - a(\eta(u))) ,$$

we denote the distribution as $\mathcal{E}_m(\eta(u), T)$. We now state and prove a proposition.

**Proposition B.8.** Let $A : \mathbb{R}^d \to \mathbb{R}^d$ be a measure isomorphism for two sets of $K + 1$ exponential family distributions, in the sense that

$$\mathcal{E}_m(\eta_a(u_i), T_a) = \mathcal{E}_m(\eta_b(u_i), T_b) \circ A^{-1}$$

Suppose that, for the first $K$ $u_i$’s, both $\eta_a(u_i)$ and $\eta_b(u_i)$ are linearly independent. Then,

$$T_b(A(z)) = L^\top T_a(z) + d,$$

almost everywhere, where $L$ is a $K \times K$ invertible matrix and $d$ is a $K$-dimensional vector not depending on $x$.

**Proof.** Fix $j = K + 1$, i.e., such that $u_j$ is not in the linearly independent subset. From Corollary B.7 and by taking logarithms, we have for each $i \neq j$,

$$\eta_a(u_i)^\top T_a(z) - a(\eta_a(u_i)) - (\eta_a(u_j)^\top T_a(z) - a(\eta_a(u_j)))$$

almost everywhere, which simplifies to

$$\eta_a(u_i) - \eta_a(u_j) = (\eta_b(u_i) - \eta_b(u_j)) - (\eta_b(u_j)^\top T_b(A(z)) - a(\eta_b(u_j)))$$

almost everywhere. $c_a$, $c_b$ are differences in the normalizing constants $a(\eta_a)$, and do not depend on $z$—we suppress the dependency on $u$ for convenience. Written in matrix form, we have

$$\begin{bmatrix}
\eta_a(u_0) - \eta_a(u_j) \\
\vdots \\
\eta_a(u_K) - \eta_a(u_j)
\end{bmatrix}^\top T_a(z) = \begin{bmatrix}
\eta_b(u_0) - \eta_b(u_j) \\
\vdots \\
\eta_b(u_K) - \eta_b(u_j)
\end{bmatrix}^\top T_b(A(z)) + c,$$

almost everywhere, where $c$ is the vector of differences $c_a - c_b$. Following [19], we will call these two matrices $L_a$ and $L_b$, noting that they are invertible since their rows are linearly
independent by assumption. Then, we obtain

\begin{align}
L_a^\top T_a(z) &= L_b^\top T_b(A(z)) + c \\
\implies T_b(A(z)) &= (L_b^{-1} L_a)^\top T_a(z) - (L_b^{-1} L_a)^\top c \\
\implies T_b(A(z)) &= L^\top T_a(z) + d,
\end{align}

almost everywhere, where \( L = L_b^{-1} L_a \) is invertible and \( d = -L^\top c \).

Identifiability of the iVAE then follows by a straight-forward application of Corollary 4.1.

**PROPOSITION 4.3.** Suppose a generative model is described by (8) with latent distributions described by (11), and that \( m \) is strictly positive. Suppose we observe at least \( K + 1 \) distinct values of \( u_i \) such that the corresponding natural parameters \( \{ \eta(u_i) \}_{i=0}^K \) are linearly independent. Then, the indeterminacy map satisfies

\[ T_b(A_{a,b}(z)) = L^\top T_a(z) + d, \]

\( \lambda_z \)-almost everywhere, where \( L \) is an invertible \( K \times K \) matrix and \( d \) is a \( K \)-dimensional vector.

**PROOF.** By Corollary 4.1 and since we do not constrain \( F \), the generator is identifiable up to the transformations described in Proposition B.8.

**B.3. Proofs for Section 4.3.** Here, we present proofs for the strong identifiability of our proposed exponential family model. These results are simply special cases of the theory developed above by setting \( P = P_{z,a} = P_{z,b} \) and where \((P_{z,a}, P_{z,b})\)-measure isomorphisms are replaced with \( P \)-measure automorphisms.

Recall that \( P_1, P_2 \) are said to be from a fixed exponential family, parametrized by its natural parameter, if the density for \( P_1 \) can be expressed as:

\[ p_1(x) = m(x) \exp(\eta_1^\top T(x) - a(\eta_1)), \]

and similarly for \( P_2 \), where both \( m \) and \( T \) are fixed. Using notation from the main text, we have \( P_1 = \mathcal{E}_{m,T}(\eta_1), P_2 = \mathcal{E}_{m,T}(\eta_2) \).

**LEMMA B.9.** Suppose \( A \) is simultaneously a \( P_1 \)-measure automorphism and \( P_2 \)-measure automorphism for \( P_1, P_2 \) from a fixed exponential family parametrized by \( \eta_1, \eta_2 \).
Suppose that \( m \) is strictly positive for this family. Then, we have

\[
(\eta_1 - \eta_2)^\top T(z) = (\eta_1 - \eta_2)^\top T(A(z)) \quad \text{a.e.}
\]

**Proof.** The expression is a direct consequence of Corollary B.7 by plugging in the exponential family densities \( p_{1,a} = p_{1,b} = p_1 \) and likewise for \( p_2 \). Taking logarithms on both sides, we have

\[
\eta_1^\top T(z) - \eta_2^\top T(z) - a(\eta_1) + a(\eta_2) = \eta_1^\top T(A(z)) - \eta_2^\top T(A(z)) - a(\eta_1) + a(\eta_2)
\]

\[\implies (\eta_1 - \eta_2)^\top T(z) = (\eta_1 - \eta_2)^\top T(A(z)) \quad \text{a.e.}\]

We can immediately apply this to obtain a characterization of exponential family automorphisms. Recall that the dimension of \( \mathcal{E}_{m,T} \) is the dimension the natural parameter vector, and equivalently the dimension of \( T(x) \).

**Proposition B.10.** Let \( \mathcal{E}_{m,T} \) be a fixed exponential family, with dimension \( K \), such that \( m \) is strictly positive. Let \( \eta_i \in \mathbb{R}^K \) for \( i = 0, 1, \ldots, K \) and suppose \( A : \mathbb{R}^d \to \mathbb{R}^d \) is a simultaneously a \( \mathcal{E}_{m,T}(\eta_i) \)-measure automorphism for each \( \eta_i \). Then, \( (T(z) - T(A(z))) \in \text{span}\{\eta_i - \eta_0\}^\perp \), almost everywhere.

**Proof.** Lemma B.9 applies to the \( K \) contrast vectors \( (\eta_i - \eta_0) \), so we have:

\[
(\eta_i - \eta_0)^\top (T(z) - T(A(z))) = 0 \quad \text{a.e.}
\]

Any vector \( v \in \text{span}(\eta_i - \eta_0) \) is of the form \( v = \sum_{i=1}^K a_i(\eta_i - \eta_0) \). Clearly,

\[
v^\top (T(z) - T(A(z))) = 0 \quad \text{a.e.},
\]

and hence \( (T(z) - T(A(z))) \in \text{span}\{\eta_i - \eta_0\}^\perp \) almost everywhere.

More useful for strong identifiability is the following result.

**Proposition B.11.** Let \( \mathcal{E}_{m,T} \) be a fixed exponential family, with dimension \( K \), such that \( m \) is strictly positive and \( T \) is injective. Suppose that \( \eta_i \in \mathbb{R}^K \), \( i = 0, 1, \ldots, K \) span \( \mathbb{R}^K \). Suppose \( A : \mathbb{R}^d \to \mathbb{R}^d \) is a simultaneously a \( \mathcal{E}_{m,T}(\eta_i) \)-measure automorphism for each \( \eta_i \). Then, \( A(z) = z \), almost everywhere.
PROOF. Without loss of generality, assume that \( \eta_0 \) is such that \( \{ \eta_i - \eta_0 \} \) forms a basis of \( \mathbb{R}^K \). By Proposition B.10, \( (T(z) - T(A(z))) \in \text{span}\{ \eta_i - \eta_0 \}^\perp = (\mathbb{R}^K)^\perp = \{0\} \). This shows that \( T(A(z)) = T(z) \) almost everywhere. If \( T \) is injective, then we have

\[
(43) \quad A(z) = z \quad \text{a.e.}.
\]

Strong identifiability as in Theorem 4.4 is now a straightforward application of the above result.

THEOREM 4.4. Let \( \mathcal{M}(\mathcal{F}, \{\mathcal{P}_e\}_{e \in \mathcal{E}}, \lambda_z) \) be the multiple environments model described in (8), with \( Z = \mathbb{R}^d \). For a subset of environments \( E^* \subset E \), with \( |E^*| = K + 1 \), fix \( P_e^z = \mathcal{E}_{m,T}(\eta_e) \) with \( m \) strictly positive and \( T \) injective in at least one dimension, and such that the corresponding parameters \( \{\eta_e\}_{e \in E^*} \) span \( \mathbb{R}^K \). Then \( \mathcal{M}(\mathcal{F}, \{\mathcal{P}_e\}_{e \in \mathcal{E}}, \lambda_z) \) is strongly identifiable.

PROOF. In this model, we have \( \mathcal{P}_e^z = \{\mathcal{E}_{m,T}(\eta_e)\} \). By Corollary 4.1, the generator is identifiable up to \( A(\mathcal{F}) \cap (\cap_e A(\{\mathcal{E}_{m,T}(\eta_e)\})) \). By Proposition B.11, \( \cap_e A(\{\mathcal{E}_{m,T}(\eta_e)\}) \) contains only functions that are equal to the identity almost everywhere, and hence the model is strongly identifiable.

B.4. Geometric characterization of iVAE indeterminacies. We can further characterize the indeterminacy set geometrically in terms of the orthogonal complements of the subspace spanned by the natural parameter vectors; see Fig. Appx.1 and Proposition B.10 for details.

PROPOSITION B.12. In the multiple environments model described in Theorem 4.4 (with \( Z = \mathbb{R}^d \)), fix a base environment with distribution \( \mathcal{N}(0, \Sigma) \) and a subset \( E^* \) of environments where \( |E^*| = d' \leq d \), with distributions \( \mathcal{N}(\mu_e, \Sigma) \). Suppose \( \{\mu_e\}_{e \in E^*} \) are linearly independent, and \( (\mu_e)_i = 0 \) for each \( e \) and \( i \notin d^* \) for some collection of dimensions \( d^* \). Then, for any indeterminacy map \( A_{a,b} \) it holds that

\[
(44) \quad (A_{a,b}(x))_{i \in d^*} = (x)_{i \in d^*} \quad \text{a.e.}
\]

PROOF. Similarly to the previous identifiability proofs, we appeal to Corollary 4.1 and analyze the shared automorphisms. For Gaussian distributions with a fixed covariance matrix...
INDETERMINACY IN LATENT VARIABLE MODELS

(a) The indeterminacy set in red with Normal means $\mu_1 = (1, 0, 0), \mu_2 = (0, 1, 0)$.

(b) The indeterminacy set (under the sufficient statistic) in red for parameter vectors $\eta_1, \eta_2$.

Fig Appx.1: a) Proposition B.12 and b) Proposition B.10, with $\mu_0 = \eta_0 = 0$. The orthogonal complement of a plane in $\mathbb{R}^3$ is the perpendicular line through the origin.

varying by its mean, we have $T(x) = x$, and $\eta_i = \mu_i$. Using the base environment we have $\mu_0 = 0$. By Proposition B.10, we have $(z - A(z)) \in \text{span}\{\mu_i\}^\perp$.

Arranging $\{\mu_i\}$ into each row of a $d' \times d$ matrix $M$, it is an elementary fact that $\text{span}\{\mu_i\}^\perp = \text{Ker}(M)$, the kernel or null-space of $M$. Furthermore, $M$ has columns of 0 corresponding to $d^*$ and linearly independent rows. Together, standard Gaussian elimination reveals that the reduced row echelon form of $M$ has the following form:

$$
\begin{bmatrix}
1 & 0 & 0 & \cdots & \mu_1 \\
0 & 1 & 0 & \cdots & \mu_2 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & \mu_{d^*}
\end{bmatrix}
\quad
(45)
$$

The corresponding null space is the space of vectors with 0 entries for the indices $d^*$. Hence, $(z - A(z)) \in \text{span}\{\mu_i\}^\perp$ implies $(A(z))_{i \in d^*} = (z)_{i \in d^*}$. □

APPENDIX C: TRIANGULAR TRANSPORT MAPS

Let $f : \mathbb{R}^d \to \mathbb{R}^d$ be a monotone increasing triangular map. This means that:

$$
\begin{bmatrix}
f_1(x_1) \\
f_2(x_1, x_2) \\
\vdots \\
f_d(x_1, \ldots, x_d)
\end{bmatrix}
\quad
(46)
$$
where each \( x_d \rightarrow f_d(x_{1:d-1}, x_d) \) is monotone increasing (hence invertible) for any \( x_{1:d-1} \).

The inverse of \( f \) is as follows:

\[
(47) \quad f^{-1}(x) = \begin{bmatrix}
    f_1^{-1}(x_1) \\
    f_2^{-1}(f_1^{-1}(x_1), x_2) \\
    \vdots \\
    f_d^{-1}(f_1^{-1}(x_1), f_2^{-1}(f_1^{-1}(x_1), x_2), \ldots, x_d)
\end{bmatrix}.
\]

This is also a monotone increasing triangular map—the inverses of monotone increasing maps are also monotone increasing. Note the map described above is lower-triangular—upper-triangular maps are analogously defined. For the purposes of this section, a triangular map refers to a lower-triangular map. As long as all maps considered are either lower, or upper triangular, the same closure properties apply.

C.1. Knöthe–Rosenblatt transports. Now, it is well-known that if \( \mu = \nu \circ f^{-1} \), where \( \mu, \nu \) have strictly positive density and \( f \) is a monotone increasing triangular map, then \( f \) is equivalent to the Knöthe–Rosenblatt (KR) transport almost everywhere. The KR transport is described recursively as follows. Let \( F_\mu(x_m|x_{1:m-1}) \) be the conditional CDF of the \( m \)-th component of \( \mu \) on the preceding components. Because \( \mu \) has strictly positive density, \( F_\mu \) is monotone increasing. Then, the \( m \)-th component of the KR transport is as follows:

\[
(48) \quad K_m(x_{1:m-1}, x_m) = F^{-1}_\nu \{ F_\mu(x_m|x_{1:m-1}) \mid K_1(x_1), \ldots, K_{m-1}(x_{1:m-1}) \}.
\]

That is, \( K_m \) sends \( x_m \) through the conditional CDF of \( \mu \) on \( x_{1:m-1} \), and back through the inverse conditional CDF of \( \nu \) on \( y_{1:m-1} = (K_1(x_1), \ldots, K_{m-1}(x_{1:m-1})) \). This CDF transform is the unique (almost everywhere) monotone increasing transport map between the 1-dimensional unique (almost everywhere) regular conditional probabilities.

It is clear that the map \( K \) defined by its components \( K_m \) is monotone increasing triangular. Since it is the unique such map transporting \( \mu \) to \( \nu \), and triangular monotone increasing maps are closed under inverses and compositions, it must be that:

- For \( K \) the KR transport from \( \mu \) to \( \nu \), \( K^{-1} \) is the KR transport from \( \nu \) to \( \mu \).
- For measures \( \mu, \nu, \pi \), if \( K_1 \) is the KR transport from \( \mu \) to \( \nu \), \( K_2 \) is the KR transport from \( \nu \) to \( \pi \), then \( K_1 \circ K_2 \) is the KR transport from \( \mu \) to \( \pi \).
Now, it is clear that if $f_a, f_b$ are KR transport, their indeterminacy map $A_{a,b}$ is also a KR transport. This drives our results from the main paper—the proofs are trivial given the observations above.

**Theorem 5.3.** Let $\mathbf{Z} = \mathbf{X} = \mathbb{R}^d$, and $\mathcal{P}^e_z = \{P^e_z\}$, where for each $e \in E$, $P^e_z \ll \lambda_z$ is any fixed probability distribution on $\mathbb{R}^d$ with strictly positive density. If $\mathcal{F}$ consists entirely of triangular monotone increasing maps, then $\mathcal{M}(\mathcal{F}, \{P^e_z\}_{e \in E}, \lambda_z)$ is strongly identifiable for any $|E| \geq 1$.

**Proof.** By Theorem 3.2, $A(\mathcal{M})$ is the set of functions equal almost everywhere to KR maps transporting between measures in $\mathcal{P}_z$. Since $\mathcal{P}_z = \{P_z\}$, $A(\mathcal{M})$ is the set of functions equal almost everywhere to the KR transport from $P_z$ to itself—the identity map. The same holds for a collection of $\{P^e_z\}_{e \in E}$ in multiple environments, hence the model is strongly identifiable.

**Proposition 5.4.** Let $\mathbf{Z} = \mathbf{X} = \mathbb{R}^d$. The ICA model with $\mathcal{M}(\mathcal{F}, P_z, \lambda_z)$ with $\mathcal{F}$ (mixing functions) consisting entirely of triangular monotone increasing maps and $\mathcal{P}_z$ fully supported distributions with independent components is identifiable up to invertible, component-wise transformations.

**Proof.** By Theorem 3.2, $A(\mathcal{M})$ is the set of functions equal almost everywhere to KR transports between measures in $\mathcal{P}_z$. Let $P_{z,a}$ and $P_{z,b}$ be two such measures, which by assumption have independent components. By its construction, it is clear that $K_m$ depends only on $x_m$ in any KR transport $K$ between $P_{z,a}$ and $P_{z,b}$. Such a map is monotone increasing and diagonal—hence an invertible, component-wise transformation.

**APPENDIX D: EXAMPLES**

**D.1. Example: Linear-Gaussian.** We present a simple example of using multiple environments, and a basis of priors, to obtain identifiability, using only linear algebra concepts. This example also provides intuition for the minimality of the number of environments. That is, for this 2-d latent space, three environments is enough to obtain strong identifiability, while two environments is insufficient.
Suppose two competing linear generative models for a random vector $X \in \mathbb{R}^{10}$ with latent vector $Z \in \mathbb{R}^2$, for data arising from three environments indexed by $e = 1, 2, 3$:

$$Z^{(e)} \sim N(\mu, I_{2 \times 2})$$
$$\epsilon \sim N(\mu, I_{10 \times 10})$$

(49) $X^{(e)} = \alpha + FZ^{(e)} + \epsilon$

(50) $X^{(e)} = \alpha + FZ^{(e)} + \epsilon$.

The left model is a single environment model, while in the right model, two of the $\mu_e$ are linearly independent, i.e., a multiple environment model. Note that the generator function here is

$$g(z) = \alpha + Fz,$$

where $F$ is a full rank $10 \times 2$ matrix, and $\alpha$ is an offset vector in data space, fixed for all environments. For each environment we have the marginal distribution under the multiple environment model:

$$X^{(e)} \sim N(\alpha + F\mu_e, FF^\top + I_{10 \times 10})$$

(52) Recall the Gaussian distribution is characterized entirely by its mean and covariance—that is, for marginal distributions parametrized by $\theta_1 = (\alpha_1, F_1), \theta_2 = (\alpha_2, F_2)$:

$$P_{\theta_1,e} = P_{\theta_2,e} \iff \alpha_1 + F_1\mu_e = \alpha_2 + F_2\mu_e, \quad F_1F_1^\top = F_2F_2^\top.$$ 

(53) To say that this model is strongly identifiable means that the right-hand-side equalities for each $e$ imply $\alpha_1 = \alpha_2$ and $F_1 = F_2$.

In the single environments model, there are the following constraints:

$$\alpha_1 + F_1\mu = \alpha_2 + F_2\mu$$

(54) $F_1F_1^\top = F_2F_2^\top$

(55) The single environments model is not identifiable. For example, let $R$ be an orthogonal (rotation) matrix, then, let $F_2 = F_1R$ and $\alpha_2 = \alpha_1 - F_1R\mu + F_1\mu$. We have

$$\alpha_2 + F_2\mu = \alpha_1 - F_1R\mu + F_1\mu + F_1R\mu = \alpha_1 + F_1\mu$$

(56) $F_2F_2^\top = F_1RR^\top F_2^\top = F_1F_1^\top$,

(57)
where the last equality is due to $R$ being an orthogonal matrix. This is a classical case of exploiting the rotational invariance of the Gaussian to construct a non-identifiable example.

Now, we analyze the multiple environment model. To be explicit, the three environments impose the following constraints in the multiple environments model:

\begin{align}
\alpha_1 + F_1 \mu_1 &= \alpha_2 + F_2 \mu_1 \\
\alpha_1 + F_1 \mu_2 &= \alpha_2 + F_2 \mu_2 \\
\alpha_1 + F_1 \mu_3 &= \alpha_2 + F_2 \mu_3 \\
F_1 F_1^\top &= F_2 F_2^\top,
\end{align}

(58) \hspace{1cm} (59) \hspace{1cm} (60) \hspace{1cm} (61)

We can show directly that these constraints imply that $\alpha_1 + F_1 z = \alpha_2 + F_2 z$. First, assume that $\mu_1$ and $\mu_2$ are the linearly independent pair. Then, taking differences,

\begin{align}
F_1 (\mu_1 - \mu_3) &= F_2 (\mu_1 - \mu_3) \\
F_1 (\mu_2 - \mu_3) &= F_2 (\mu_2 - \mu_3) \\
F_1 F_1^\top &= F_2 F_2^\top.
\end{align}

(62) \hspace{1cm} (63) \hspace{1cm} (64)

Written in matrix form, the first two constraints read

\begin{align}
F_1 M &= F_2 M \implies F_1 = F_2,
\end{align}

(65)

since $\mu_1 - \mu_3$ and $\mu_2 - \mu_3$ remain linearly independent, and hence $M$ is invertible. It immediately follows from the original constraints that $\alpha_1 = \alpha_2$ also.

The above analysis showed that, for identifiability, a single environment was insufficient, while three environments was adequate. This begs the question, what about two environments? In other words, is the three environment constraint minimal?

Consider a model with two environments with means $\mu_1$, $\mu_2$. By the arguments above, it imposes the following constraints:

\begin{align}
\alpha_1 + F_1 \mu_1 &= \alpha_2 + F_2 \mu_1 \\
\alpha_1 + F_1 \mu_2 &= \alpha_2 + F_2 \mu_2 \\
F_1 F_1^\top &= F_2 F_2^\top.
\end{align}

(66) \hspace{1cm} (67) \hspace{1cm} (68)

Can we construct an non-identifiable example? Let $F_2 = F_1 R$, $\alpha_2 = \alpha_1 - F_1 R \mu_1 + F_1 \mu_1$ as in the single-environment case. Clearly, these satisfy the first and third constraint for any
orthogonal matrix $R$. We aim to find a specific rotation matrix that also satisfies the second constraint. Observe that:

\begin{equation}
\alpha_2 + F_2 \mu_2 = \alpha_1 - F_1 R \mu_1 + F_1 \mu_1 + F_1 R \mu_2
\end{equation}

\begin{equation}
= \alpha_1 + F_1 \mu_1 + F_1 R (\mu_2 - \mu_1).
\end{equation}

Let $x$ be a vector orthogonal to $\mu_2 - \mu_1$, standardized such that $\|x\|^2 = \|\mu_2 - \mu_1\|^2$. Consider

\begin{equation}
R = \frac{1}{\|\mu_2 - \mu_1\|^2} \begin{bmatrix}
| & | & | & | \\
\mu_2 - \mu_1 & x & 1 & 0 \\
| & | & | & |
\end{bmatrix}
\begin{bmatrix}
| & | & | & | \\
1 & 0 & | & | \\
0 & -1 & | & | \\
| & | & | & |
\end{bmatrix}
\begin{bmatrix}
| & | & | & | \\
\mu_2 - \mu_1 & x & 1 & 0 \\
| & | & | & |
\end{bmatrix}^T.
\end{equation}

This is the eigendecomposition of an orthogonal matrix (it is the product of orthogonal matrices) with eigenvalues 1 and $-1$, and corresponding eigenvectors $\mu_2 - \mu_1$ and $x$. Since it is an eigenvector, we have $R(\mu_2 - \mu_1) = \mu_2 - \mu_1$.\footnote{R is essentially a rotation matrix with axis $(\mu_2 - \mu_1)$.} Then, we have

\begin{equation}
\alpha_2 + F_2 \mu_2 = \alpha_1 + F_1 \mu_1 + F_1 \mu_2 - F_1 \mu_1 = \alpha_1 + F_1 \mu_2,
\end{equation}

which satisfies the second constraint as desired. This shows that three environments are required, and hence minimal for strong identifiability of this model.

Note that such a construction will not work for the three-environment model. For three environments, the rotation has to satisfy both

\begin{equation}
R(\mu_3 - \mu_1) = \mu_3 - \mu_1
\end{equation}

\begin{equation}
R(\mu_2 - \mu_1) = \mu_2 - \mu_1,
\end{equation}

that is, the eigenspace of $R$ associated to the eigenvalue 1 spans $\mathbb{R}^2$, i.e., it is the identity.

\section{D.2. Linear, non-Gaussian ICA.}

Consider a generative model (Equation (2)) with $Z = \mathbb{R}^{d_z}$ and $X = \mathbb{R}^{d_x}$. Assume $d_x \geq d_z$. Let the generator parameter space be $\mathcal{F} = \{ A \in \mathbb{R}^{d_x \times d_z}; rank(A) = d_z \}$. That is, the generators are full-rank linear transformations, and hence injective. Let the prior parameter space be

\begin{equation}
\mathcal{P}_z = \{ p(z) = \prod_{i=1}^{d_z} p_i(z); p_i \text{ are non-Gaussian, and not a point mass} \},
\end{equation}

e.g., probability distributions on $\mathbb{R}^{d_z}$ with a density, and the density factorizes as independent, non-Gaussian components.
The identifiability of this problem was first studied in [5]. In their analysis, identifiability is established up to pre-multiplication of a diagonal matrix and a permutation. That is, for generators $F_a, F_b \in \mathcal{F}$ with $P_{z,a}, P_{z,b} \in \mathcal{P}_z$, if the marginal distributions of $X$ match, then $F_a = F_b \Lambda P$, where $\Lambda$ is an invertible diagonal matrix and $P$ is a permutation matrix.

Under our framework, i.e., Lemma 3.1, we must have that $P_{z,b} = P_{z,a} \circ A_{a,b}^{-1}$, where $F_a = F_b \circ A_{a,b}$. Using our framework, we now show that $A_{a,b} = \Lambda P$ as above. The identifiability result obtained in [5] rests on the following result (restated and re-proved to match our notation):

**Theorem D.1 (Theorem 10, [5]).** Let $z$ be a random vector with factorized density. Let $x = Cz$, such that $x$ also has factorized density. Then, $z_j$ is non-Gaussian if the $j$-th column has at most one non-zero entry.

**Proof.** We require Theorem 19 from [5].

**Lemma D.2 ([5], Darmois’ Theorem).** Define two random variables $Z_1$ and $Z_2$ as

$$Z_1 = \sum_i a_i z_i, \quad Z_2 = \sum_i b_i z_i,$$

where $z_i$ are independent random variables, i.e., their joint distribution factorizes. Then, if $Z_1$ and $Z_2$ are independent, all variables $z_j$ for which $a_j b_j \neq 0$ are Gaussian.

Now, let $z$ be a random vector with factorized density and $x = Cz$, where $x$ has factorized density also. Note that this implies any $x_i, x_k$ are independent for $i \neq k$. We have that

$$x_i = \sum_j C_{ij} z_j, \quad x_k = \sum_j C_{kj} z_j,$$

and hence by Lemma D.2, if $z_j$ is non-Gaussian, it must be that $C_{ij} C_{kj} = 0$. This holds for each $i \neq k$, and hence, the $j$-th column has at most one non-zero entry.

---

7In the original analysis, the model is fit according to a criteria maximizing the independence between components, and also one component of the prior is allowed to be Gaussian. For simplicity, we will simply study the implications of matching observational marginal distributions (i.e., maximum likelihood) and where all prior components are non-Gaussian.
Recall the definition of $\mathcal{P}_z$ is such that any prior must factorize and be non-Gaussian. Then, Theorem D.1 implies that

(78)
$$\mathcal{A}(\mathcal{P}_z) \cap \mathbb{R}^{d_x \times d_z} = \{ A \in \mathbb{R}^{d_x \times d_z} \mid A \text{ has no column with more than one nonzero element} \}.$$ 

That is, any linear isomorphisms between two priors must have no column with more than one nonzero element. Now, note that for any $A_{a,b} \in \mathcal{A}(\mathcal{F})$, we have

(79)
$$A_{a,b} = f_b^{-1} \circ F_a,$$

where $f_b^{-1}$ is the restriction of the linear map represented by the pseudoinverse $F_b^\dagger$ to the range of $\mathcal{F}$. By Lemma B.2, $A_{a,b}$ is an invertible linear map and hence full rank. Finally, we conclude that for any $A_{a,b} \in \mathcal{A}(\mathcal{F}) \cap \mathcal{A}(\mathcal{P})$, $A_{a,b}$ must have exactly one nonzero element in each column. We can then apply a permutation $P$ such that $PA_{a,b} = \Lambda$, where $\Lambda$ is diagonal. Finally, we obtain $A_{a,b} = P^\top \Lambda$, where $P^\top$ is a permutation matrix and $\Lambda$ is diagonal and invertible.