Independent Mechanism Analysis in GPLVMs

Abstract

Independence is a common assumption when modeling generative processes. Independent Mechanism Analysis (IMA) relies on the Independent Causal Mechanisms (ICM) principle to formulate non-statistical independence by measuring the decoder Jacobian's column-orthogonality. This work is based on observations of the same column-orthogonality in GPLVMs and shows how additive and stationary kernels give rise to independent mechanisms in expectation. To handle the probabilistic nature of GPLVMs, we provide an upper bound for the orthogonality measure under specific kernel conditions. By connecting IMA and GPLVMs, our paper makes the first step to elucidate a useful inductive bias in GPLVMs for recovering the true latent factors, which we demonstrate in our synthetic experiments.

1. Introduction

Independence is a prevalent assumption in machine learning with most works relying on statistical independence (Hyvärinen and Pajunen, 1999; Kingma and Welling, 2014). The ICM principle (Peters et al., 2018) conceptually formulates independence of "modules" that correspond to nature's mechanisms. It was translated into a non-statistical independence notion in Independent Mechanism Analysis (IMA) (Gresele et al., 2021), which defines independent mechanisms in generative models (or decoders, i.e., the mapping from latent factors to observations) by having a column-orthogonal Jacobian. The proposed regularized log-likelihood objective provably rules out spurious solutions in the task of learning the true latent factors. Buchholz et al. (2022) proved identifiability for conformal maps, where the Jacobian columns have equal norms, and showed local identifiability for the IMA function class. Reizinger et al. (2022) connected IMA to Variational Autoencoders (VAEs) (Kingma and Welling, 2014) in the limiting case of isotropic observation noise with diminishing variance. By observing that Gaussian Process Latent Variable Models (GPLVMs) (Lawrence, 2005) also often possess the same column orthogonality, we connect GPLVMs to independent mechanisms. Our **contributions** are:

- We describe the kernel properties necessary to satisfy the non-statistical independence of IMA in priors of functions of GPLVMs;
- Similar to Ghosh (2022), we provide an upper bound on IMA's orthogonality measure and show that under specific kernel choices, the IMA principle holds approximately;
- We demonstrate in toy experiments how the learned latent space in GPLVMs resembles the true one.

2. Background

Notation We are interested in generative models with decoder maps $\boldsymbol{f} : \mathcal{Z} \to \mathcal{X}$ and their Jacobians $\mathbf{J}_{\boldsymbol{f}} = \mathbf{J}_{\boldsymbol{f}}(\boldsymbol{z})$, with $\mathcal{Z}$ and $\mathcal{X}$ being the latent and observation spaces with

dimensions d and D, respectively. We denote $\mathbf{J}_{\boldsymbol{f}} := \partial \boldsymbol{f}/\partial \boldsymbol{z} \in \mathbb{R}^{D \times d}$ such that $(\mathbf{J}_{\boldsymbol{f}})_{ij} := \partial \boldsymbol{f}_i^k/\partial z_j^k$, i.e., the ith row and j^{th} column gives the partial derivative of the ith dimension of $\boldsymbol{f}$ for the latent dimension j (for a given sample k, which we will omit for brevity). The observations are denoted by matrix $\mathbf{X} \in \mathbb{R}^{n \times D}$ and the corresponding latent variables as $\mathbf{Z} \in \mathbb{R}^{n \times d}$. The ith dimension of the kth observation is given by x_i^k.

2.1. Independent Mechanism Analysis (IMA)

Observations $\boldsymbol{x}$ are often modeled as a mixture of latent factors, $\boldsymbol{x} = \boldsymbol{f}(\boldsymbol{z})$. Representation learning then learns an unmixing $\boldsymbol{g}$ such that the recovered components $\boldsymbol{y} = \boldsymbol{g}(\boldsymbol{x})$ recover the true ones up to tolerable ambiguities (Bengio et al., 2013; Khemakhem et al., 2020)—which is impossible for nonlinear $\boldsymbol{f}$ without further constraints (Hyvärinen and Pajunen, 1999; Locatello et al., 2019). Gresele et al. (2021) constrain the mixing function class in an approach termed Independent Mechanism Analysis (IMA), postulating that latent components influence the observations "independently" through the partial derivatives $\partial \boldsymbol{f}/\partial z_k$. This is equivalent to an orthogonality condition on the decoder Jacobian's columns. While identifiability only holds for a subset of this model class (Buchholz et al., 2022), IMA provably rules out the most common counterexamples to identifiability, and empirical results show that it helps recover the ground-truth latent factors (Gresele et al., 2021; Sliwa et al., 2022; Reizinger et al., 2022). IMA optimizes the regularized log-likelihood: $\mathcal{L}_{\mathrm{IMA}}(\boldsymbol{f}, \boldsymbol{z}) := \log p_{\boldsymbol{\theta}}(\boldsymbol{x}) - \lambda \cdot c_{\mathrm{IMA}}(\boldsymbol{f}, \boldsymbol{z})$ where the regularizer $c_{\mathrm{IMA}}(\boldsymbol{f}, \boldsymbol{z})$ encourages column-orthogonality of $\mathbf{J}_{\boldsymbol{f}}(\boldsymbol{z})$. $c_{\mathrm{IMA}}(\boldsymbol{f}, \boldsymbol{z})$ and its expectation $C_{\mathrm{IMA}}(\boldsymbol{f}, p(\boldsymbol{z}))$ are defined as

$$c_{\mathrm{IMA}}(\boldsymbol{f}, \boldsymbol{z}) = \sum_k \log \left\| \frac{\partial \boldsymbol{f}}{\partial z_k}(\boldsymbol{z}) \right\| - \log |\mathbf{J}_{\boldsymbol{f}}(\boldsymbol{z})|; \quad C_{\mathrm{IMA}}(\boldsymbol{f}, p(\boldsymbol{z})) = \mathbb{E}_{p(\boldsymbol{z})}[c_{\mathrm{IMA}}(\boldsymbol{f}, \boldsymbol{z})]. \quad (1)$$

2.2. Gaussian Process Latent Variable Models (GPLVMs)

Gaussian Processes (GPs) are stochastic processes over real-valued functions (Rasmussen and Williams, 2006), which provide a Bayesian non-parametric framework for inference. GPLVMs (Lawrence, 2005) model the mapping between latent variables $\boldsymbol{z}$ and observed data $\boldsymbol{x}$ with GP priors. Independent GPs model each of the D observed dimensions as $x_i^k = f_i(\boldsymbol{z}^k) + \varepsilon_i^k$, where $\varepsilon_i^k \sim \mathcal{N}(0; \beta^{-1}\mathbf{I}_d)$. When a GP prior is placed over $\mathbf{X}$ and when $\boldsymbol{f} = \{\boldsymbol{f}_i\}_{i=1}^D : \boldsymbol{f}_i := \boldsymbol{f}_i(\boldsymbol{z}) + \varepsilon_i$ is marginalized, the likelihood for $\mathbf{X}$ is given by:

$$p(\mathbf{X}|\mathbf{Z}) = \prod_{i=1}^D p(\boldsymbol{x}_i|\mathbf{Z}); \qquad p(\boldsymbol{x}_i|\mathbf{Z}) = \mathcal{N}(\boldsymbol{x}_i|\mathbf{0}, \mathcal{K} + \beta^{-1}\mathbf{I}_n), \qquad (2)$$

where $\mathcal{K} \in \mathbb{R}^{n \times n}$ is the GP's covariance matrix, given by the kernel $(\mathcal{K})_{ij} := k(\boldsymbol{z}^i; \boldsymbol{z}^j)$.

GP derivatives. By the linearity of differentiation, the derivative of a GP is, in a mean-squared sense, a GP (Rasmussen and Williams, 2006, Sec. 9.4); i.e., $\mathcal{GP}(\mathbf{0}, \mathcal{K}(\boldsymbol{z}))' = \mathcal{GP}(\mathbf{0}, \mathcal{K}(\boldsymbol{z})'')$, provided that the kernel function is at least twice differentiable (Papoulis and Unnikrishna Pillai, 2002). This derivative process corresponds to the partial derivative $\partial \boldsymbol{f}/\partial \boldsymbol{z}$. This also holds for differentiable mean functions; however, w.l.o.g., we assume zero mean, which implies $\mathbb{E}[\mathbf{J}_{\boldsymbol{f}}|\boldsymbol{z}] = \mathbf{0}_{D \times d}$ over the function priors. For a given $\boldsymbol{z}$ (dropping k and using only $\boldsymbol{f}$ without subscript), the derivative GP's covariance function is given by a

$d \times d$–dimensional matrix

$$\left[\mathcal{K}\left(\boldsymbol{z}\right)''\right]_{eg} = \left[\mathbb{E}\left[\mathbf{J}_{\boldsymbol{f}}^{\top}\mathbf{J}_{\boldsymbol{f}}|\boldsymbol{z}\right]\right]_{eg} = \mathrm{Cov}\left[\frac{\partial \boldsymbol{f}}{\partial z_e}, \frac{\partial \boldsymbol{f}}{\partial z_g}\right] = \frac{\partial^2 k\left(\boldsymbol{z}; \boldsymbol{z}\right)}{\partial z_e \partial z_g}. \tag{3}$$

Additive and stationary kernels. Additive kernels of oth order[1] Duvenaud et al. (2011) associate a one-dimensional *base kernel* $k(z_i, z_i')$ to each dimension of $\boldsymbol{z}$ and compose the kernel function as the weighted sum of the products of each combination of $\leq o$ kernels. For first-order additive kernels, this means $\mathcal{K}\left(\boldsymbol{z}\right) := \sum_{i=1}^{d} k(z_i, z_i')$. Stationary kernels can be expressed as a function of the distance $z_i - z_i'$, and for isotropic kernels such as the Radial Basis Function (RBF) kernel, k only depends on $|z_i - z_i'|$.

3. Theoretical Results

We are interested in characterizing when GPLVMs satisfy the IMA principle, i.e., when the columns of the prior decoder Jacobian are zero in expectation: $C_{\mathrm{IMA}}(\boldsymbol{f}, p\left(\boldsymbol{z}\right)) = 0$. Our analysis focuses on kernel choice, for which we express $c_{\mathrm{IMA}}(\boldsymbol{f}, \boldsymbol{z})$ as the left KL-measure of diagonality (Alyani et al., 2017) of the matrix $\mathbf{J}_{\boldsymbol{f}}^{\top}\mathbf{J}_{\boldsymbol{f}}$, which depends on $\boldsymbol{z}$. $\mathbf{J}_{\boldsymbol{f}}^{\top}\mathbf{J}_{\boldsymbol{f}}$ has a Wishart distribution with D degrees of freedom, $\mathbf{J}_{\boldsymbol{f}}^{\top}\mathbf{J}_{\boldsymbol{f}} \sim \mathcal{W}_d\left(\mathbf{A}; D\right)$, where the scale matrix $\mathbf{A}$ needs to be diagonal for IMA to hold over the function priors. I.e., $\left[\mathbb{E}\left[\mathbf{J}_{\boldsymbol{f}}^{\top}\mathbf{J}_{\boldsymbol{f}}\right]\right]_{i \neq j} = 0$. These off-diagonal entries correspond to the expectation of the cross-derivatives from (3), connecting IMA to the kernel—note that our claim is about the marginal variance, i.e., when $k\left(\boldsymbol{z}; \boldsymbol{z}'\right) : \boldsymbol{z} = \boldsymbol{z}'$. Since $\mathbb{E}\left[\mathbf{J}_{\boldsymbol{f}}^{\top}\mathbf{J}_{\boldsymbol{f}}\right] = \mathbb{E}\left[\mathbb{E}\left[\mathbf{J}_{\boldsymbol{f}}^{\top}\mathbf{J}_{\boldsymbol{f}}|\boldsymbol{z}\right]\right]$, the inner expectation yields

$$\mathbb{E}\left[\mathbf{J}_{\boldsymbol{f}}^{\top}\mathbf{J}_{\boldsymbol{f}}|\boldsymbol{z}\right]_{ij} = \sum_{k=1}^{D} \mathbb{E}\left[(\mathbf{J}_{\boldsymbol{f}})_{ki}(\mathbf{J}_{\boldsymbol{f}})_{kj}\right] = \sum_{k=1}^{D} \mathrm{Cov}\left[\frac{\partial f_k}{\partial z_i}, \frac{\partial f_k}{\partial z_j}\right] = \frac{\partial^2 k\left(\boldsymbol{z}; \boldsymbol{z}\right)}{\partial z_i \partial z_j} \tag{4}$$

Thus, $\left[\mathbb{E}\left[\mathbf{J}_{\boldsymbol{f}}^{\top}\mathbf{J}_{\boldsymbol{f}}\right]\right]_{i \neq j} = 0$ when the expectation of the cross-derivative of $k\left(\boldsymbol{z}; \boldsymbol{z}\right)$ is zero. We leverage this insight in two steps: first, we show how to design GPLVMs such that the above expectation is diagonal: by choosing first-order additive or stationary kernels (Prop. 1). Then, we bound $C_{\mathrm{IMA}}(\boldsymbol{f}, p\left(\boldsymbol{z}\right))$ to show that (Prop. 2).

Proposition 1 $\left(\partial_{ij}^2 k = 0 \iff k = \sum_i k_i(z_i)\right)$ *The cross-derivatives of* (4) *are zero if and only if the marginal variance can be decomposed into a sum of terms that depend at most on one latent coordinate z_i.*[2]

Proof $\partial_{ij}^2 k\left(\boldsymbol{z}; \boldsymbol{z}\right)$ denotes the cross derivative of $k\left(\boldsymbol{z}; \boldsymbol{z}\right)$ w.r.t. z_i, z_j, and A, B some functionals.
$\implies$: By assumption, the cross-derivative $\partial_{ij}^2 k\left(\boldsymbol{z}; \boldsymbol{z}\right)$ is zero. we integrate twice: by z_i, then by z_j, which gives rise to the additive functionals A, B. Integration by z_i would mean that

---

1. We focus on $o = 1$
2. "At most" implies that besides first-order additive kernels, stationary kernels are also included since they can be expressed as the distance between the two points. Since we consider $k\left(\boldsymbol{z}; \boldsymbol{z}\right)$, the distance is 0, yielding a constant term

the resulting additive functional can depend on any $z_{j\neq i}$. Since $i \neq j$ are arbitrary, z_i, z_j cannot be in the same functional, so only one latent component remains:

$$\partial_j k\left(\boldsymbol{z}; \boldsymbol{z}\right) = A'(z_j) \tag{5}$$

$$k\left(\boldsymbol{z}; \boldsymbol{z}\right) = \int A'(z_j)dz_j = A(z_j) + B(z_i), \tag{6}$$

which shows that $k\left(\boldsymbol{z}; \boldsymbol{z}\right)$ factorizes into functions of single latent coordinates (or constant terms), i.e., when the kernel is the sum of base kernels depending on at most one coordinate. $\Longleftarrow$: By assumption, the kernel decomposes into base kernels depending on at most one latent coordinate, i.e., $k\left(\boldsymbol{z}; \boldsymbol{z}\right) = \sum_{i=1}^d k_i(\boldsymbol{z}; \boldsymbol{z})$. Differentiating by z_i and then by z_j yields

$$\partial_i k\left(\boldsymbol{z}; \boldsymbol{z}\right) = \sum_{i=1}^d \partial_i\ k_i(\boldsymbol{z}; \boldsymbol{z}) = \partial_i\ k_i(\boldsymbol{z}; \boldsymbol{z}) \tag{7}$$

$$\partial_{ij}^2 k\left(\boldsymbol{z}; \boldsymbol{z}\right) = \partial_{ij}\ k_i(\boldsymbol{z}; \boldsymbol{z}) = 0, \tag{8}$$

which is zero since each k_i depends only on z_i. ∎

Prop. 1 characterizes the kernel family that fulfill the necessary requirement for the IMA principle (if the kernel is also twice-differentiable). However, our result only implies that the expected value of $\mathbf{J}_{\boldsymbol{f}}^\top \mathbf{J}_{\boldsymbol{f}}$ is diagonal. Since a GPLVM defines a distribution over both $\boldsymbol{f}$ and $\mathbf{J}_{\boldsymbol{f}}$, this might imply that though $\mathbb{E}\left[\mathbf{J}_{\boldsymbol{f}}^\top \mathbf{J}_{\boldsymbol{f}}\right]$ is diagonal, IMA is not satisfied for each $\boldsymbol{f}$ drawn from the $\mathcal{GP}$.

Proposition 2 $(D \to \infty | d \implies C_{\mathbf{IMA}}(\boldsymbol{f}, p\left(\boldsymbol{z}\right)) \to 0)$ *If a GPLVM has a kernel that is twice-differentiable and has zero cross-derivatives, then $D \to \infty \implies C_{\mathrm{IMA}}(\boldsymbol{f}, p\left(\boldsymbol{z}\right)) \to 0$ for a given d[3]. Note that this statement assumes the prior distribution over $\boldsymbol{f}$ (i.e. this is before conditioning on any data point or inducing point).*

Proof

We formulate $C_{\mathrm{IMA}}(\boldsymbol{f}, p\left(\boldsymbol{z}\right))$ as the expected left KL-measure of diagonality of $\mathbf{J}_{\boldsymbol{f}}^\top \mathbf{J}_{\boldsymbol{f}}$ (Alyani et al., 2017):

$$C_{\mathrm{IMA}}(\boldsymbol{f}, p\left(\boldsymbol{z}\right)) = \mathbb{E}\left[\log\left|\mathrm{diag}\left(\mathbf{J}_{\boldsymbol{f}}^\top \mathbf{J}_{\boldsymbol{f}}\right)\right| - \log\left|\mathbf{J}_{\boldsymbol{f}}^\top \mathbf{J}_{\boldsymbol{f}}\right|\right], \tag{9}$$

where $\mathbf{J}_{\boldsymbol{f}}^\top \mathbf{J}_{\boldsymbol{f}}$ has a Wishart distribution, $\mathcal{W}_d\left(\mathbf{A}; D\right)$, where $\mathbf{A}$ is the matrix with elements $a_{ij} = \partial_{ij}^2 k\left(\boldsymbol{z}; \boldsymbol{z}\right)$. Together with the expression for the expectation of the log-determinant of a Wishart distribution (Bishop and Nasrabadi, 2006, App. B, p. 693), the observation that the diagonals of $\mathbf{J}_{\boldsymbol{f}}^\top \mathbf{J}_{\boldsymbol{f}}$ are $a_{ii} \cdot \chi_D^2$–distributed (Rao et al., 1973, 8b.2, p. 535), and that of the expectation of a $\log(\chi_D^2)$ distribution (Pav, 2015); $C_{\mathrm{IMA}}(\boldsymbol{f}, p\left(\boldsymbol{z}\right))$ becomes

$$= \sum_{i=1}^d \left[\psi\left(\frac{D}{2}\right) - \psi\left(\frac{D+1-i}{2}\right)\right] + \log\left|\mathrm{diag}\left(\mathbf{A}\right)\right| - \log\left|\mathbf{A}\right| \tag{10}$$

---

3. Note that d does not have to be fixed, as long as it is restricted to a function of D such that the upper bound collapses

Where the digamma $\psi(k)$ and multivariate digamma $\psi_p(k)$ functions are, respectively

$$\psi(k) = \frac{d}{dk} \log(\Gamma(k)) = \frac{\Gamma'(k)}{\Gamma(k)}; \qquad \psi_p(k) = \sum_{i=1}^{p} \psi\left(k + \frac{1-i}{2}\right). \tag{11}$$

$\mathbf{A}$ is diagonal, when $\partial_{ij}^2 k(\boldsymbol{z}; \boldsymbol{z}) = 0$ for $i \neq j$, which means that the last two terms cancel, and we can bound the expression with

$$C_{\text{IMA}}(\boldsymbol{f}, p(\boldsymbol{z})) \leq d\left[\psi\left(\frac{D}{2}\right) - \psi\left(\frac{D+1-d}{2}\right)\right], \tag{12}$$

since $\psi(k)$ is strictly increasing and concave. This upper bound goes to zero for a fixed d as $D \to \infty$ due to the continuity of ψ. This can also be seen through the limiting behaviour of the digamma function for large real arguments, i.e., $\psi(k) \approx \log(k) - 1/2k$, yielding

$$\approx d\left[\log\left(\frac{D}{D+1-d}\right) + \frac{1-d}{D(D+1-d)}\right]. \tag{13}$$

∎

Notably, Prop. 2 aligns with the result of Ghosh (2022), which shows that as D grows for a given d, $C_{\text{IMA}}(\boldsymbol{f}, p(\boldsymbol{z}))$ can be upper bounded—Ghosh (2022) assumes that the columns of $\mathbf{J}_f$ are drawn i.i.d. from a spherically invariant distribution. Since the prerequisite for Prop. 2 is to have a kernel with zero cross-derivatives, our result might suggest an unexpected consequence of kernel choice: since IMA is beneficial for recovering the true latent factors, GPLVMs might also have such properties, at least for high-dimensional observations. Lastly, given the kernel choice, the upper bound does not depend on any kernel hyper-parameters.

Invariances in GPLVMs. Since C_{IMA} is the expectation over $\boldsymbol{z}$, Prop. 2 that when the symmetries (invariances) of the latent distribution and the kernel align, then the expectation will be zero, e.g., when a standard normal prior accompanies the linear additive kernel. Our work suggests that these invariances might also play a role in recovering the ground-truth latents in GPLVMs.

4. Experiments

Setup. We generate 500 samples via the Möbius transform using (Stimper et al., 2021), where $\boldsymbol{z}$ is uniformly distributed in $[0; 1]^d$. For visualization, we set $d = D = 2$ (the Möbius transform is a bijective map). We use (GPy, 2012), RBF kernel, and the L-BFGS (Liu and Nocedal, 1989) optimizer with 5 seeds, 5 restarts, and monitor C_{IMA}. Besides vanilla GPLVMs, we also experiment with sparse ones since they are faster to train.

Results. Figure 1 replicates (Gresele et al., 2021, Fig. 4 (Top)) to visualize the relation of the inferred and true latent factors (the estimated latents are transformed by the cumulative distribution function of the uniform distribution for the figure). From left to right, we plot the true latent factors, the observations, and the reconstructed latents for the vanilla and sparse GPLVMs, respectively (we plot the representations of the models with the lowest C_{IMA}). Since $d = D = 2$; thus, Prop. 2 gives the loose bound of $\psi(1) - \psi(1/2) \approx 1.386$, we use $\mathbf{J}_f^\top \mathbf{J}_f | \boldsymbol{z}$ instead of sampling from the corresponding Wishart distribution, which yields $C_{\text{IMA}} \approx 1\text{e}{-}2$.

Figure 1: **From left to right:** true latent factors; observations generated by the Möbius transform; reconstructed latents (GPLVM); reconstructed latents (sparse GPLVM)

5. Discussion

Limitations. To visualize the latent space structure, our experiments are restricted to $d = D = 2$, which is a practically less relevant, though theoretically widely-employed scenario when studying the recovery of the true latent factors (Hyvärinen and Pajunen, 1999; Gresele et al., 2021). However, our results suggest that when the IMA condition (approximately) holds in GPLVM, then they elicit beneficial properties for recovering the true latent factors, though this requires further investigation.

Conclusion. Our work connects kernel choice in GPLVMs to Independent Mechanism Analysis (IMA) (Gresele et al., 2021) by stating that zero cross-derivatives—such as in first-order additive and stationary kernels—are necessary for the IMA condition to hold in the prior over the functions of the GPLVM. Furthermore, we upper bound IMA's (non-statistical) independence measure based on the observation and latent dimensions and show that for a given latent dimensionality, increasing the observation dimension makes the bound go to zero. The connection betwee IMA and GPLVMs possibly explains the observation of practitioners that the decoder Jacobian in GPLVMs can have orthogonal columns. Our experimental results on synthetic data suggest that the orthogonality of the Jacobian columns is beneficial for learning the true latent factors in GPLVMs.

References

Khaled Alyani, Marco Congedo, and Maher Moakher. Diagonality measures of Hermitian positive-definite matrices with application to the approximate joint diagonalization problem. *Linear Algebra and its Applications*, 528:290–320, September 2017. ISSN 0024-3795. doi: 10.1016/j.laa.2016.08.031. URL https://www.sciencedirect.com/science/article/pii/S0024379516303834.

Y. Bengio, A. Courville, and P. Vincent. Representation learning: A review and new perspectives. *IEEE Trans. Pattern Anal. Mach. Intell.*, 35(8):1798–1828, August 2013. ISSN 0162-8828, 2160-9292. doi: 10.1109/tpami.2013.50. URL https://doi.org/10.1109/tpami.2013.50.

Christopher M Bishop and Nasser M Nasrabadi. *Pattern recognition and machine learning*, volume 4. Springer, 2006.

Simon Buchholz, Michel Besserve, and Bernhard Schölkopf. Function Classes for Identifiable Nonlinear Independent Component Analysis. page 25, 2022. URL https://arxiv.org/abs/2208.06406.

David K Duvenaud, Hannes Nickisch, and Carl Rasmussen. Additive gaussian processes. *Advances in neural information processing systems*, 24, 2011.

Shubhangi Ghosh. Independent Mechanism Analysis in High-Dimensional Observation Spaces. Master's thesis, June 2022. URL https://www.research-collection.ethz.ch/handle/20.500.11850/591418?show=full. Accepted: 2023-01-11T08:54:06Z.

GPy. GPy: A gaussian process framework in python. http://github.com/SheffieldML/GPy, 2012.

Luigi Gresele, Julius von Kügelgen, Vincent Stimper, Bernhard Schölkopf, and Michel Besserve. Independent mechanism analysis, a new concept? *arXiv:2106.05200 [cs, stat]*, June 2021. URL http://arxiv.org/abs/2106.05200. arXiv: 2106.05200.

Aapo Hyvärinen and Petteri Pajunen. Nonlinear independent component analysis: Existence and uniqueness results. *Neural Networks*, 12(3):429–439, April 1999. ISSN 0893-6080. doi: 10.1016/S0893-6080(98)00140-3. URL https://www.sciencedirect.com/science/article/pii/S0893608098001403.

Ilyes Khemakhem, Diederik Kingma, Ricardo Monti, and Aapo Hyvarinen. Variational Autoencoders and Nonlinear ICA: A Unifying Framework. In *International Conference on Artificial Intelligence and Statistics*, pages 2207–2217. PMLR, June 2020. URL http://proceedings.mlr.press/v108/khemakhem20a.html. ISSN: 2640-3498.

Diederik P. Kingma and Max Welling. Auto-Encoding Variational Bayes. *arXiv:1312.6114 [cs, stat]*, May 2014. URL http://arxiv.org/abs/1312.6114. arXiv: 1312.6114.

Neil Lawrence. Probabilistic non-linear principal component analysis with gaussian process latent variable models. *Journal of machine learning research*, 6(11), 2005.

Dong C Liu and Jorge Nocedal. On the limited memory bfgs method for large scale optimization. *Mathematical programming*, 45(1-3):503–528, 1989.

Francesco Locatello, Stefan Bauer, Mario Lucic, Gunnar Raetsch, Sylvain Gelly, Bernhard Schölkopf, and Olivier Bachem. Challenging Common Assumptions in the Unsupervised Learning of Disentangled Representations. In *International Conference on Machine Learning*, pages 4114–4124. PMLR, May 2019. URL http://proceedings.mlr.press/v97/locatello19a.html. ISSN: 2640-3498.

Athanasios Papoulis and S Unnikrishna Pillai. *Probability, random variables and stochastic processes*. 2002.

Steven E Pav. Moments of the log non-central chi-square distribution. *arXiv preprint arXiv:1503.06266*, 2015.

Jonas Peters, Dominik Janzing, and Bernhard Schölkopf. Elements of causal inference: foundations and learning algorithms. *Journal of Statistical Computation and Simulation*, 88(16):3248–3248, November 2018. ISSN 0094-9655, 1563-5163. doi: 10.1080/00949655.2018.1505197. URL https://www.tandfonline.com/doi/full/10.1080/00949655.2018.1505197.

Calyampudi Radhakrishna Rao, Calyampudi Radhakrishna Rao, Mathematischer Statistiker, Calyampudi Radhakrishna Rao, and Calyampudi Radhakrishna Rao. *Linear statistical inference and its applications*, volume 2. Wiley New York, 1973.

Carl Edward Rasmussen and Christopher K. I. Williams. *Gaussian processes for machine learning*. Adaptive computation and machine learning. MIT Press, Cambridge, Mass, 2006. ISBN 978-0-262-18253-9. OCLC: ocm61285753.

Patrik Reizinger, Luigi Gresele, Jack Brady, Julius Von Kügelgen, Dominik Zietlow, Bernhard Schölkopf, Georg Martius, Wieland Brendel, and Michel Besserve. Embrace the Gap: VAEs Perform Independent Mechanism Analysis. October 2022. URL https://openreview.net/forum?id=G4GpqX4bKAH.

Joanna Sliwa, Shubhangi Ghosh, Vincent Stimper, Luigi Gresele, and Bernhard Schölkopf. Probing the Robustness of Independent Mechanism Analysis for Representation Learning, July 2022. URL http://arxiv.org/abs/2207.06137. arXiv:2207.06137 [cs, stat].

Vincent Stimper, Luigi Gresele, Joanna Sliwa, and Adrián Javaloy. Independent Mechanism Analysis repository. https://github.com/lgresele/independent-mechanism-analysis, 2021.

Acronyms

IMA Independent Mechanism Analysis

GP Gaussian Process
GPLVM Gaussian Process Latent Variable Model

i.i.d. independent and identically distributed

ICM Independent Causal Mechanisms

KL Kullback-Leibler Divergence

RBF Radial Basis Function

VAE Variational Autoencoder

Nomenclature

Independent Mechanism Analysis
$C_{\textbf{IMA}}$ global IMA contrast
$\boldsymbol{y}$ reconstructed sources
$\mathcal{L}_{\textbf{IMA}}$ IMA loss function
$c_{\textbf{IMA}}$ local IMA contrast

Gaussian Processes
$\mathcal{GP}$ Gaussian Process
$\mathcal{K}$ $n \times n$ covariance matrix of a GP
k kernel function

Variational Autoencoders
$\boldsymbol{\theta}$ parameters of the decoder $p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})$
$\boldsymbol{g}$ inverse decoder
$p_{\boldsymbol{\theta}}(\boldsymbol{x})$ marginal likelihood
$p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})$ conditional distribution of the decoded samples of the VAE, mapping $\boldsymbol{z} \mapsto \boldsymbol{x}$, parametrized by $\boldsymbol{\theta}$
$\boldsymbol{f}$ decoder map $\mathcal{Z} \rightarrow \mathcal{X}$
f decoder map component
n number of samples

Algebra

$\boldsymbol{0}$ a vector of zeros
$\mathbf{I}$ identity matrix
$\mathbf{J}$ Jacobian matrix

Latents
$\boldsymbol{z}$ latent vector
$\mathbf{Z}$ latent matrix of $\mathbb{R}^{n \times d}$
$\mathcal{Z}$ latents
d dimensionality of the latent space $\mathcal{Z}$
z latent single component

Observations
D dimensionality of the observation space $\mathcal{X}$
$\boldsymbol{x}$ observation vector
$\mathbf{X}$ observation matrix of $\mathbb{R}^{n \times D}$
$\mathcal{X}$ observation space
x observation single component

Probability theory
$\mathcal{N}$ normal distribution
$\mathcal{W}$ Wishart distribution