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MultiVae: A Python package for Multimodal Variational Autoencoders on Partial Datasets

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DOI: 10.xxxxxx/draft

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Submitted: 01 January 1970
Published: unpublished

In partnership with

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This article and software are linked with research article DOI 10.3847/xxxxx <- update this with the DOI from AAS once you know it., published in the Astrophysical Journal <- The name of the AAS journal..

Summary

In recent years, there has been a major boom in the development of multimodal machine learning models. Among open topics, representation (fusion) and generation of multimodal data are very active fields of research. Recently, Multimodal Variational Autoencoders (VAEs) have been attracting growing interest for both tasks, thanks to their versatility, scalability, and interpretability as probabilistic latent variable models. They are also particularly interesting models in the *partially observed* setting, as most of them can learn even with missing data. This last point makes them particularly interesting for research fields such as the medical field, where missing data are commonplace (Antelmi et al., 2019; Lawry Aguila et al., 2023).

We present MultiVae, an open-source Python library for bringing together unified implementations of multimodal VAEs. It has been designed for easy, customizable use of these models on fully or partially observed data. This library also facilitates the development and benchmarking of new algorithms by integrating several benchmark datasets, a variety of evaluation metrics and tools for monitoring and sharing models.

Multimodal Variational Autoencoders

In Multimodal Machine Learning, two goals are generally targeted: (1) Learn a shared representation from multiple modalities; (2) Learn to generate one missing modality given the ones that are available.

Multimodal Variational Autoencoders aim at solving both issues at the same time. These models learn a latent representation z of all modalities in a lower dimensional common space and learn to *decode* z to generate any modality (Suzuki & Matsuo, 2022). Let $X = (x_1, x_2, ...x_M)$ contain M modalities. In the VAE setting, we suppose that the generative process behind the observed data is the following:

$$z \sim p(z) \qquad \forall 1 \leq i \leq M, x_i|z \sim p_\theta(x_i|z) \tag{1}$$

where $p(z)$ is a prior distribution that is often fixed, and $p_\theta(x_i|z)$ are called *decoders* and are parameterized by neural network. Typically, $p_\theta(x_i|z) = \mathcal{N}(x_i; \mu_\theta(z), \sigma_\theta(z))$ where $\mu_\theta, \sigma_\theta$ are neural networks. We aim to learn these *decoders* that translate z into the high dimensional data x_i. At the same time, we aim to learn an *encoder* $q_\phi(z|X)$ that map observations to the latent space. $q_\phi(z|X)$ is also parameterized by a neural network. Derived from variational inference (Kingma & Welling, 2014), the VAE objective writes:

$$\mathcal{L}(X) = \mathbb{E}_{q_\phi(z|X)}\left(\sum_i \ln(p_\theta(x_i|z))\right) - KL(q_\phi(z|X)|p(z))$$

The first term is a reconstruction loss and the second term can be seen as a regularization term that avoids overfitting. A typical training of a multimodal VAE consists in encoding the

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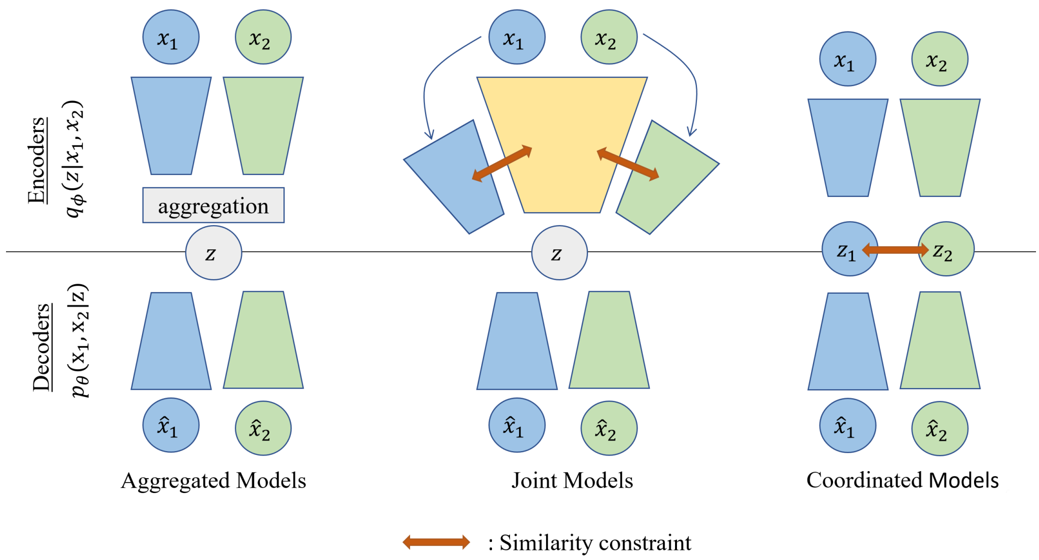
data with the encoder, reconstructing each modality with the decoders and taking a gradient step to optimize the loss $\mathcal{L}(X)$.

Most multimodal VAEs differ in how they construct the encoder $q_\phi(z|X)$. In the figure below, we summarize several approaches: *Aggregated models* (Shi et al., 2019; Sutter et al., 2021; Wu & Goodman, 2018) use a mean or a product operation to aggregate the information coming from all modalities, where *Joint models* (Senellart et al., 2023; Suzuki et al., 2016; Vedantam et al., 2018) use a neural network taking all modalities as input. Finally *coordinated models* (Tian & Engel, 2019; Wang et al., 2017a) use different latent spaces but add a constraint term in the loss to force them to be similar.



In our library, we implement all these approaches in an unified and modular way.

Aggregated models offer a natural way of learning on incomplete datasets: for an incomplete sample X, we use only the available modalities to encode the data and compute the loss. However, except in MultiVae, there doesn't exist an implementation of these models that can be used on incomplete datasets in a straightforward manner.

Data Augmentation

Another application of these models is Data Augmentation (DA): from sampling latent codes z and decoding them, *fully synthetic multimodal* samples can be generated to augment a dataset. DA has been proven useful in many data-intensive deep learning applications (Chadebec et al., 2023). In a dedicated module `multivae.samplers`, we propose different ways of sampling latent codes z to further explore the generative abilities of these models.

Statement of need

Although multimodal VAEs have interesting applications in different fields, the lack of easy-to-use and verified implementations might hinder applicative research. With MultiVae, we offer unified implementations, designed to be easy to use by non-specialists and even on incomplete data. In order to propose reliable implementations of each method, we tried to reproduce, whenever possible, a key result from the original paper. Some works similar to ours have grouped together model implementations: the Multimodal VAE Comparison Toolkit (Sejnova et al., 2024) includes 4 models and the Pixyz(Masahiro Suzuki & Matsuo, 2023) library contains 2 multimodal models. The work closest to ours and released while we were developping our library is `multi-view-ae` (Aguila et al., 2023), which contains a dozen of models. We compare in a summarizing table below, the different features of each work. Our library complements what already exists: our API is quite different compared to previous work, the models implemented are not all the same, and for those we have in common, our implementation offers additional parameterization options. Indeed, for each model, we've made sure to offer great flexibility on parameters and to include all implementation details present in the original codes. Our library also offers additional features: **compatibility with incomplete data**, which we consider essential for real-life applications, and a range of tools dedicated to research and development of new algorithms: benchmark datasets, metrics modules and samplers, for testing and analyzing models.

List of models and features

In the Table below, we list available models and features, and compare to previous work. This symbol (✓*) indicates that the implementation include additional options.

Models/ Features	Ours	(Aguila et al., 2023)	(Sejnova et al., 2024)
JMVAE (Suzuki et al., 2016)	✓*	✓	
MVAE(Wu & Goodman, 2018)	✓*	✓	✓
MMVAE(Shi et al., 2019)	✓*	✓	✓
MoPoE(Sutter et al., 2021)	✓*	✓	✓
DMVAE(Lee & Pavlovic, 2021)	✓	✓*	✓
MVTCAE(Hwang et al., 2021)	✓	✓	
MMVAE+(Palumbo et al., 2023)	✓*	✓	
CMVAE(Palumbo et al., 2024)	✓		
Nexus(Vasco et al., 2022)	✓		
CVAE(Kingma & Welling, 2014)	✓		
MHVAE(Dorent et al., 2023)	✓		
TELBO(Vedantam et al., 2018)	✓		
JNF(Senellart et al., 2023)	✓		
CRMVAE(Suzuki & Matsuo, 2023)	✓		
MCVAE(Antelmi et al., 2019)		✓	
mAAE		✓	
DVCCA(Wang et al., 2017b)		✓	
mWAE		✓	
mmJSD(Sutter et al., 2020)		✓	
gPoE(Lawry Aguila et al., 2023)		✓	
Support of Incomplete datasets	✓		
GMM Sampler	✓		
MAF Sampler, IAF Sampler	✓		
Metrics: Likelihood, Coherences, FIDs, Reconstruction, Clustering	✓		
Ready-to-use Datasets	✓		✓
Model sharing via Hugging Face	✓		

An important difference in our user-interface, is that we handle all training and model parameters within python dataclasses while (Sejnova et al., 2024; **?**) uses independant `YAML` configuration files.

Code quality and documentation

Our code is available on Github (https://github.com/AgatheSenellart/MultiVae) and Pypi and we provide a full online documentation at (https://multivae.readthedocs.io/en/latest/). The main features are illustrated through tutorials made available either as notebooks or scripts allowing users to get started easily. To further showcase how to use our library for research applications, we provide detailed case studies here.

Acknowledgements

We are grateful to the authors of all the initial implementations of the models included in MultiVae.

References

Aguila, A. L., Jayme, A., Montaña-Brown, N., Heuveline, V., & Altmann, A. (2023). Multi-view-AE: A python package for multi-view autoencoder models. *Journal of Open Source Software*, *8*(85), 5093. https://doi.org/10.21105/joss.05093

Antelmi, L., Ayache, N., Robert, P., & Lorenzi, M. (2019). *Sparse multi-channel variational autoencoder for the joint analysis of heterogeneous data*. *97*, 302–311. https://proceedings.mlr.press/v97/antelmi19a.html

Chadebec, C., Thibeau-Sutre, E., Burgos, N., & Allassonnière, S. (2023). Data augmentation in high dimensional low sample size setting using a geometry-based variational autoencoder. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, *45*(3), 2879–2896. https://doi.org/10.1109/TPAMI.2022.3185773

Dorent, R., Haouchine, N., Kogl, F., Joutard, S., Juvekar, P., Torio, E., Golby, A. J., Ourselin, S., Frisken, S., Vercauteren, T., Kapur, T., & Wells, W. M. (2023). Unified brain MR-ultrasound synthesis using multi-modal hierarchical representations. In *Medical image computing and computer assisted intervention – MICCAI 2023* (pp. 448–458). Springer Nature Switzerland. https://doi.org/10.1007/978-3-031-43999-5_43

Hwang, H., Kim, G.-H., Hong, S., & Kim, K.-E. (2021). Multi-view representation learning via total correlation objective. *Advances in Neural Information Processing Systems*, *34*, 12194–12207.

Kingma, D. P., & Welling, M. (2014). *Auto-Encoding Variational Bayes*. arXiv. http://arxiv.org/abs/1312.6114

Lawry Aguila, A., Chapman, J., & Altmann, A. (2023). *Multi-modal variational autoencoders for normative modelling across multiple imaging modalities*. 425–434. https://doi.org/10.1007/978-3-031-43907-0_41

Lee, M., & Pavlovic, V. (2021). *Private-shared disentangled multimodal VAE for learning of latent representations*. 1692–1700. https://doi.org/10.1109/CVPRW53098.2021.00185

Masahiro Suzuki, T. K., & Matsuo, Y. (2023). Pixyz: A python library for developing deep generative models. In *Advanced Robotics* (No. 0; Vol. 0, pp. 1–16). Taylor & Francis. https://doi.org/10.1080/01691864.2023.2244568

Palumbo, E., Daunhawer, I., & Vogt, J. E. (2023). *MMVAE+: ENHANCING THE GENERATIVE QUALITY OF MULTIMODAL VAES WITHOUT COMPROMISES*.

Palumbo, E., Manduchi, L., Laguna, S., Chopard, D., & Vogt, J. E. (2024). *Deep generative clustering with multimodal diffusion variational autoencoders*. https://openreview.net/forum?id=k5THrhXDV3

Sejnova, G., Vavrecka, M., Stepanova, K., & Taniguchi, T. (2024). *Benchmarking multimodal variational autoencoders: CdSprites+ dataset and toolkit*. https://arxiv.org/abs/2209.03048

Senellart, A., Chadebec, C., & Allassonnière, S. (2023). Improving multimodal joint variational autoencoders through normalizing flows and correlation analysis. *arXiv Preprint arXiv:2305.11832*.

Shi, Y., Siddharth, N., Paige, B., & Torr, P. H. S. (2019). Variational Mixture-of-Experts Autoencoders for Multi-Modal Deep Generative Models. *arXiv:1911.03393 [Cs, Stat]*. http://arxiv.org/abs/1911.03393

Sutter, T. M., Daunhawer, I., & Vogt, J. E. (2020). Multimodal generative learning utilizing jensen-shannon-divergence. *CoRR*, *abs/2006.08242*. https://arxiv.org/abs/2006.08242

Sutter, T. M., Daunhawer, I., & Vogt, J. E. (2021). Generalized Multimodal ELBO. *ICLR*.

Suzuki, M., & Matsuo, Y. (2022). A survey of multimodal deep generative models. *Advanced Robotics*, *36*(5-6), 261–278. https://doi.org/10.1080/01691864.2022.2035253

Suzuki, M., & Matsuo, Y. (2023). *Mitigating the limitations of multimodal VAEs with coordination-based approach*. https://openreview.net/forum?id=Rn8u4MYgeNJ

Suzuki, M., Nakayama, K., & Matsuo, Y. (2016). Joint Multimodal Learning with Deep Generative Models. *arXiv:1611.01891 [Cs, Stat]*. http://arxiv.org/abs/1611.01891

Tian, Y., & Engel, J. (2019). Latent Translation: Crossing Modalities by Bridging Generative Models. *ArXiv*.

Vasco, M., Yin, H., Melo, F. S., & Paiva, A. (2022). Leveraging hierarchy in multimodal generative models for effective cross-modality inference. *Neural Networks*, *146*, 238–255.

Vedantam, R., Fischer, I., Huang, J., & Murphy, K. (2018). Generative Models of Visually Grounded Imagination. *arXiv:1705.10762 [Cs, Stat]*. http://arxiv.org/abs/1705.10762

Wang, W., Yan, X., Lee, H., & Livescu, K. (2017b). *Deep Variational Canonical Correlation Analysis*. arXiv. https://doi.org/10.48550/arXiv.1610.03454

Wang, W., Yan, X., Lee, H., & Livescu, K. (2017a). *Deep Variational Canonical Correlation Analysis*. arXiv. https://doi.org/10.48550/arXiv.1610.03454

Wu, M., & Goodman, N. (2018). Multimodal Generative Models for Scalable Weakly-Supervised Learning. *Advances in Neural Information Processing Systems*, *31*. https://proceedings.neurips.cc/paper/2018/hash/1102a326d5f7c9e04fc3c89d0ede88c9-Abstract.html