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

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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 in *partially observed* settings, as most can be trained even with missing data. This last point makes them particularly suited for the medical field, where available datasets are often incomplete (Antelmi et al., 2019; Lawry Aguila et al., 2023).

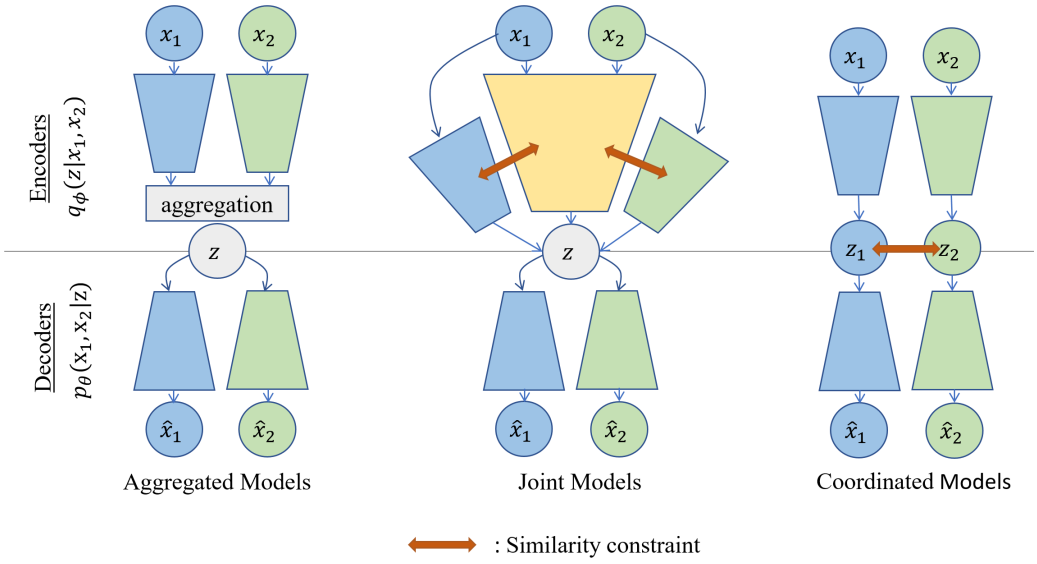
We present MultiVae, an open-source Python library bringing together unified implementations of multimodal VAEs. It has been designed for easy and customizable use of these models on fully or partially observed data. This library also facilitates the development and benchmarking of new algorithms by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

Multimodal Variational Autoencoders

Two main goals are commonly pursued in Multimodal Machine Learning: (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 each modality.
Let $X = (x_1, x_2, ...x_M)$ contain M modalities. In the VAE setting, we define an *encoder* distribution $q_\phi(z|X)$ projecting the observations to the latent space, and decoders distributions $(p_\theta(x_i|z))_{1\leq i\leq M}$ translating the latent code z back to the observations. Those distributions are parameterized by neural networks that are trained to minimize an objective function derived from variational inference. See (Kingma & Welling, 2014) to learn more about the VAE framework and (Suzuki & Matsuo, 2022) for a survey on multimodal VAEs.

A key differentiator of multimodal VAEs relies in the choice of the encoder $q_\phi(z|X)$. As illustrated in the figure below, they can be categorized into three main groups: *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., 2017) use different latent spaces while adding a constraint term in the loss to force them to be similar.



We designed our library MultiVae with the aim to implement all the approaches in a unified yet modular way.

Notably, aggregated models offer a natural way of *learning* on incomplete datasets: for an incomplete sample X, the encoding z and the objective function can be computed using only available modalities. However, except in our library MultiVae, there does not exist an implementation of these models that can be used on incomplete datasets in a straightforward manner. We propose a convenient way to handle missing modalities using *masks* in the loss computation of each aggregated model.

Data Augmentation

Another application of VAEs is Data Augmentation (DA): from sampling new latent codes z and decoding them with trained models, *fully synthetic multimodal* samples can be generated to augment a dataset. This approach has been successfully used with unimodal VAEs to augment datasets for data-intensive deep learning applications (Chadebec et al., 2023). However, the use of similar sampling techniques with multimodal VAEs remains largely unexplored. In our library, we provide a module `multivae.samplers` with popular sampling strategies 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 accessible even for non-specialists. In order to provide reliable implementations, we reproduced, whenever possible, a key result from the original paper. Related software packages 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 most closely related work, released while we were developing 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 differs and complements existing software packages as follows: 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 options. Indeed, for each model, we made sure to offer great flexibility on parameters' choices 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, **samplers** to boost the generative abilities of models, and a range of tools dedicated to research and development such **benchmark datasets** and **metrics**. We implement the most commonly used metrics in a modular way to easily evaluate any model.

List of Models and Features

In the table below, we list available models and features, and compare to previous work. Symbol (✓*) indicates that the implementation includes 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., 2017)		✓	
DCCAE(Wang et al., 2015)		✓	
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}	✓		
Benchmark Datasets	✓		✓
Model sharing via Hugging Face	✓		

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/). Our code is unit-tested with a code coverage of 94%. 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* in the documentation.

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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. *The Eleventh International Conference on Learning Representations*. https://openreview.net/forum?id=sdQGxouELX

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., Arora, R., Livescu, K., & Bilmes, J. (2015). On deep multi-view representation learning. In F. Bach & D. Blei (Eds.), *Proceedings of the 32nd international conference on machine learning* (Vol. 37, pp. 1083–1092). PMLR. https://proceedings.mlr.press/v37/wangb15.html

Wang, W., Yan, X., Lee, H., & Livescu, K. (2017). *Deep Variational Canonical Correlation Analysis*. 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